

ONLINE SEARCH REQUEST FORM

2-355

USER DARTON

SERIAL NUMBER 244863

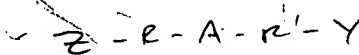
ART UNIT 124

PHONE 44710

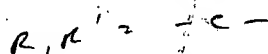
DATE 3/21/95

Please give a detailed statement of requirements. Describe as specifically as possible the subject matter to be searched. Define any terms that may have special meaning. Give examples or relevant citations, authors, or keywords, if known.

You may include a copy of the broadest and or relevant claim(s).

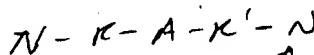


Z, Y = cyclic polyamine having 9-20 ring members + 3-6 N atoms



A = aromatic or heterocyclic group

OR this:



↑
cyclic atoms
in 9-20 member rings

Bridge Gary

STAFF USE ONLY

COMPLETED

SEARCHER

ONLINE TIME

(in minutes)

TOTAL TIME

(in minutes)

SYSTEMS

☒ CAS ONLINE

☐ DARC/QUESTEL

☐ DIALOG

☐ SDC

☐ OTHER

3-25-95

JIM DARTON

62 82

3

=>
=> d his 17-

(FILE 'CA' ENTERED AT 13:36:51 ON 25 MAR 95)

L7 37 S BRIDGER G?/AU
L8 2 S L7 AND (HIV OR AIDS OR HTLV OR IMMUNODEFICIENCY)
L9 1 S L7 AND CYCLIC
L10 2 S L8 OR L9

=> d all

L10 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS
AN 120:30786 CA
TI Linked heterocyclic polyamines with activity against HIV
IN **Bridger, Gary James**; Padmanabhan, Sreenivasan; Skerlj,
Renato Tony; Thornton, David Michael
PA Johnson Matthey P.L.C., UK
SO PCT Int. Appl., 66 pp.
CODEN: PIXXD2
PI WO 9312096 A1 930624
DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 92-GB2334 921216
PRAI GB 91-26677 911216
DT Patent
LA English
IC ICM C07D257-02
ICS C07D255-02; C07D259-00; C07D401-14; C07D409-14
CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
OS MARPAT 120:30786
AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 =
(un)substituted alk. chain or heteroatom-contg. chain; Y, Z =
cyclic polyamine moieties having 9-32 ring members and 3-8 N
atoms in the ring spaced by .gtoreq.2 C atoms from each other] or
their acid addn. salts or metal complexes are prepd. and
demonstrated viricidal activity against HIV-1 and
HIV-2. Thus, 1,1'-[1,4-phenylenebis(methylene)]bis-1,4,8,11-
tetraazacyclotetradecane was prepd. and demonstrated 50% inhibitory
concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory
concn. against HIV-2 of <0.01 .mu.g/mL in an assay
employing infected MT-4 cells.
ST AIDS treatment prepn heterocyclic polyamine; HIV
virucide prepn heterocyclic polyamine; tetraazacyclotetradecane
prepn HIV viricidal agent; virustat prepn
tetraazacyclotetradecane
IT Virucides and Virustats
(heterocyclic polyamines)
IT Virus, animal
(human immunodeficiency 1, inhibition of, heterocyclic
polyamines for)
IT Virus, animal
(human immunodeficiency 2, inhibition of, heterocyclic
polyamines for)
IT 151191-32-1 151191-33-2 151191-34-3 151191-35-4 151191-36-5
(HIV viricidal activity of)
IT 7440-50-8DP, Copper, 1,4-phenylenebismethylene bis

tetraazacyclotetradecane complexes 7440-66-6DP, Zinc,
1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes
110078-44-9P 110078-46-1DP, copper and zinc complexes

133587-10-7P	133587-11-8P	151190-72-6P	151190-73-7P
151190-74-8P	151190-75-9P	151190-76-0P	151190-80-6P
151190-81-7P	151190-85-1P	151190-87-3P	151190-91-9P
151190-93-1P	151190-94-2P	151190-95-3P	151190-96-4P
151190-97-5P	151190-98-6P	151190-99-7P	151191-02-5P
151191-03-6P	151191-05-8P	151191-06-9P	151191-08-1P
151191-09-2P	151191-12-7P	151191-14-9P	151191-15-0P
151191-17-2P	151191-18-3P	151191-20-7P	151191-21-8P
151191-24-1P	151191-25-2P	151191-26-3P	151191-27-4P
151191-28-5P	151191-29-6P	151191-30-9P	151191-31-0P
151191-37-6P	151191-38-7P	151191-39-8P	

(prepn. and HIV viricidal activity of)

IT 19417-58-4P, 1,4-Benzenedipropanol 58791-49-4P 60023-32-7P
63134-93-0P 70364-29-3P 92339-07-6P 105355-16-6P
145617-64-7P 151190-69-1P 151190-70-4P 151190-71-5P
151190-77-1P 151190-79-3P 151190-82-8P 151190-83-9P
151190-84-0P 151190-86-2P 151190-88-4P 151190-89-5P
151190-92-0P 151191-00-3P 151191-01-4P 151191-04-7P
151191-07-0P 151191-10-5P 151191-11-6P 151191-13-8P
151191-16-1P 151191-19-4P 151191-22-9P

(prepn. and reaction of, in prepn. of heterocyclic HIV
viricidal agents)

IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-
Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3,
.alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2,
Carbethoxymethylene)triphenylphosphorane 1198-37-4,
2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane
7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4
39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1
104395-69-9 110078-46-1 134457-14-0 151190-78-2 151191-23-0

(reaction of, in prepn. of heterocyclic HIV viricidal
agents)

=> fil reg ;d 151190-77-1

FILE 'REGISTRY' ENTERED AT 13:39:08 ON 25 MAR 95

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STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

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ANSWER 1 REGISTRY COPYRIGHT 1995 ACS

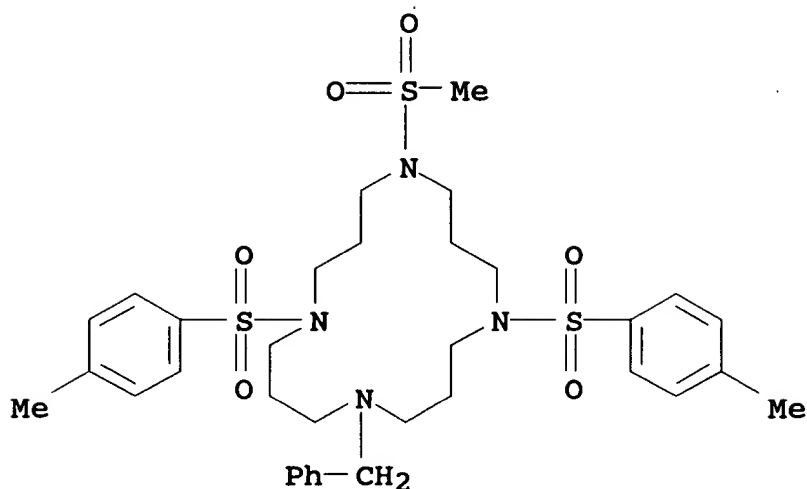
RN 151190-77-1 REGISTRY

CN 1,5,9,13-Tetraazacyclohexadecane, 1,9-bis[(4-methylphenyl)sulfonyl]-
5-(methylsulfonyl)-13-(phenylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C34 H48 N4 O6 S3

SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

=> fil req ;d 151190-94-2

FILE 'REGISTRY' ENTERED AT 13:39:35 ON 25 MAR 95

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TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when conducting SmartSELECT searches.

ANSWER 1 REGISTRY COPYRIGHT 1995 ACS

RN 151190-94-2 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,10-phenanthroline-2,9-diylbis(methylene)]bis- (9CI) (CA INDEX NAME)

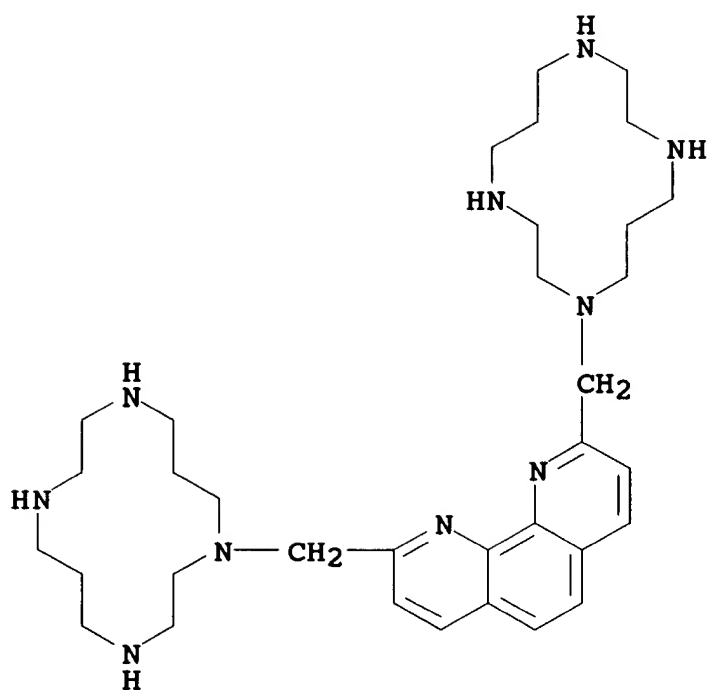
FS 3D CONCORD

MF C34 H56 N10

CI COM

SR CA

LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

=>

=>

=> fil ca

FILE 'CA' ENTERED AT 13:40:04 ON 25 MAR 95

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FILE COVERS 1967 - 18 Mar 1995 (950318/ED) VOL 122 ISS 12

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=>

=> d l10 all

L10 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS

AN 120:30786 CA

TI Linked heterocyclic polyamines with activity against HIV

IN **Bridger, Gary James**; Padmanabhan, Sreenivasan; Skerlj,
Renato Tony; Thornton, David Michael

PA Johnson Matthey P.L.C., UK

SO PCT Int. Appl., 66 pp.

CODEN: PIXXD2

PI WO 9312096 A1 930624

DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AI WO 92-GB2334 921216

PRAI GB 91-26677 911216

DT Patent

LA English

IC ICM C07D257-02

ICS C07D255-02; C07D259-00; C07D401-14; C07D409-14

CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

OS MARPAT 120:30786

AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 =
(un)substituted alk. chain or heteroatom-contg. chain; Y, Z =

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concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory
concn. against HIV-2 of <0.01 .mu.g/mL in an assay
employing infected MT-4 cells.

ST **AIDS** treatment prepn heterocyclic polyamine; **HIV**
virucide prepn heterocyclic polyamine; tetraazacyclotetradecane
prepn HIV viricidal agent; virustat prepn
tetraazacyclotetradecane

IT Virucides and Virustats
(heterocyclic polyamines)

IT Virus, animal
(human **immunodeficiency** 1, inhibition of, heterocyclic
polyamines for)

IT Virus, animal
(human immunodeficiency 2, inhibition of, heterocyclic
polyamines for)

IT 151191-32-1 151191-33-2 151191-34-3 151191-35-4 151191-36-5
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110078-44-9P 110078-46-1DP, copper and zinc complexes
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151190-81-7P 151190-85-1P 151190-87-3P 151190-91-9P
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151190-97-5P 151190-98-6P 151190-99-7P 151191-02-5P
151191-03-6P 151191-05-8P 151191-06-9P 151191-08-1P
151191-09-2P 151191-12-7P 151191-14-9P 151191-15-0P
151191-17-2P 151191-18-3P 151191-20-7P 151191-21-8P
151191-24-1P 151191-25-2P 151191-26-3P 151191-27-4P
151191-28-5P 151191-29-6P 151191-30-9P 151191-31-0P
151191-37-6P 151191-38-7P 151191-39-8P
(prepn. and HIV viricidal activity of)

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151190-77-1P 151190-79-3P 151190-82-8P 151190-83-9P
151190-84-0P 151190-86-2P 151190-88-4P 151190-89-5P
151190-92-0P 151191-00-3P 151191-01-4P 151191-04-7P
151191-07-0P 151191-10-5P 151191-11-6P 151191-13-8P
151191-16-1P 151191-19-4P 151191-22-9P
(prepn. and reaction of, in prepn. of heterocyclic HIV
viricidal agents)

IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-
Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3,
.alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2,
Carbethoxymethylene)triphenylphosphorane 1198-37-4,
2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane
7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4
39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1
104395-69-9 110078-46-1 134457-14-0 151190-78-2 151191-23-0
(reaction of, in prepn. of heterocyclic HIV viricidal
agents)

=> d 110 all 2

L10 ANSWER 2 OF 2 CA COPYRIGHT 1995 ACS
AN 118:80485 CA
TI Preparation of polyaza(cyclo)alkanes as antiviral compounds
IN Schwartz, David Aaron; Bridger, Gary
PA Johnson Matthey PLC, UK
SO PCT Int. Appl., 26 pp.
CODEN: PIXXD2
PI WO 9216494 A1 921001 ✓
DS W: AU, CA, FI, HU, JP, KR, NO, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE
AI WO 92-GB438 920311
PRAI GB 91-5489 910315
DT Patent
LA English
IC ICM C07C211-14
ICS C07D257-02; A61K031-13; A61K031-395
CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 28
OS MARPAT 118:80485
AB Title compds. Z(A)nY (Z, Y = 9 to 32-membered poly(hetero)alkyl chain, -poly(hetero)cycloalkyl moiety, each Z, Y having 3-8 heteroatoms selected from N, O, S such that at least 1 of Z, Y is the above chain; A = linking atom or group; n = 0-6), their salts metal complexes, are prepd. against HIV in std. tests. H2N(CH2)CO2H was xl-tosylated, the product esterified with N-hydroxysuccinimide, the ester treated with 1,2,3,4-meso-tetraaminobutane, the tetraamido-tetratosylate treated with borane. THF complex and the product in HBR/AcOH was heated at 100.degree. for 48 h to give meso-1,2,3,4-tetrakis(N-1,3-diaminopropyl)butane (I). In a std. in vitro test I against both HIV-1 and HIV-1 had a selectivity index (ratio of CD50 and ED50) of >13 compared with AZT >125.
ST tetrakisdiaminopropylbutate prepn virucide HIV;
tetraazacyclotetradecylbenzomethyl bis prepn virucide HIV
IT Virus, animal
(human immunodeficiency 1, infection with, treatment of, tetrakis(diaminopropyl)butane and tetraazacyclotetradecylbenzenemethylbis for)
IT Virus, animal
(human immunodeficiency 2, infection with, treatment of, tetrakis(diaminopropyl)butane and tetraazacyclotetradecylbenzenemethylbis for)
IT 42908-33-8P 145617-61-4P 145617-62-5P 145617-63-6P
145617-64-7P 145617-65-8P 145617-66-9P 145617-67-0P
145617-68-1P 145617-69-2P
(prepn. and reaction of, in prepn. of HIV virucides)
IT 145617-56-7P 145617-57-8P 145617-58-9P 145617-59-0P
145617-60-3P
(prepn. of, as HIV virucide)
IT 107-95-9, 3-Aminopropanoic acid 112-24-3 623-24-5 10563-26-5,
N,N'-Bis(3-aminopropyl)ethylenediamine 74676-47-4 92902-03-9
104395-69-9
(reaction of, in prepn. of HIV virucides)

=>

=> fil reg;d 145617-64-7

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STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

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TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

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ANSWER 1 REGISTRY COPYRIGHT 1995 ACS

RN 145617-64-7 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1-[[4-(bromomethyl)phenyl]methyl]-
4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

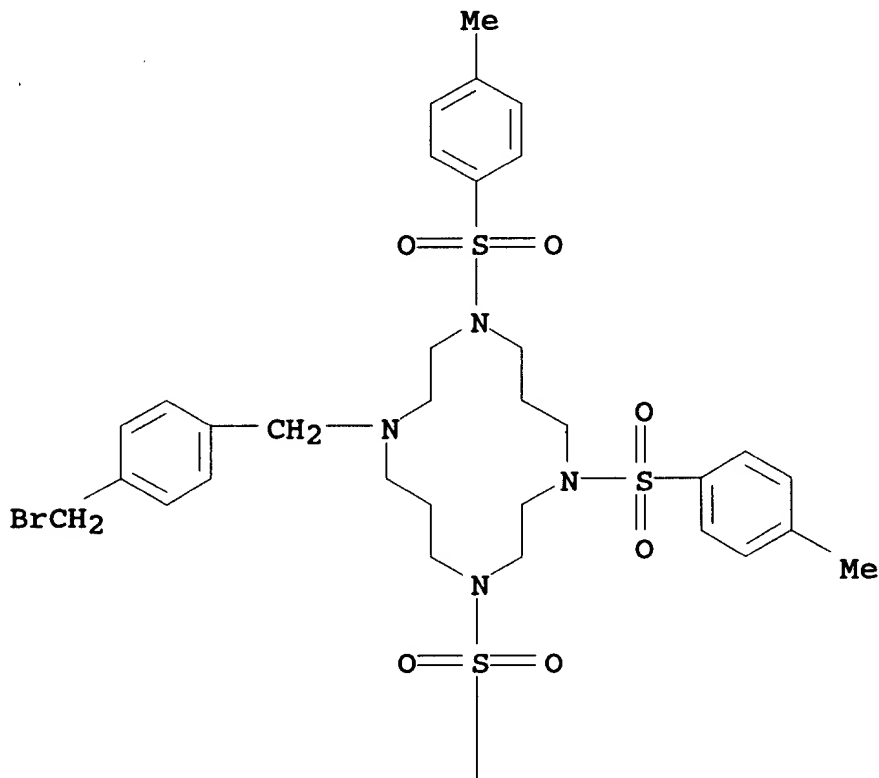
FS 3D CONCORD

MF C39 H49 Br N4 O6 S3

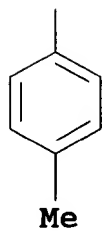
SR CA

LC STN Files: CA

PAGE 1-A



PAGE 2-A



2 REFERENCES IN FILE CA (1967 TO DATE)

=> fil reg

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=>

=> d que 128

L11 STR

N 1 N 3 N 5

NODE ATTRIBUTES:

NSPEC IS R AT 1

NSPEC IS R AT 3

NSPEC IS R AT 5

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L13 STR

N—C—Cy—C—N

1 2 3 4 5

NODE ATTRIBUTES:

NSPEC IS R AT 1

NSPEC IS R AT 5

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 3

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L17 STR

Hy—C—Cy—C—Hy

1 2 3 4 5

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS HIQ AT 1

GGCAT IS UNS AT 3
GGCAT IS HIQ AT 5
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M4 C M3 N AT 1
ECOUNT IS M4 C M3 N AT 5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L19 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L22 SCR 1840 AND 1996 AND 140 AND 1607 AND 1236
L23 SCR 1840 AND 1996 AND 140 AND 1607 AND 1363
L28 308 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L17 AND L19 AND
(L22 OR L23)

=> fil ca
FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95
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FILE COVERS 1967 - 18 Mar 1995 (950318/ED) VOL 122 ISS 12

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SmartSELECT searches with large numbers of terms.

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(FILE 'REGISTRY' ENTERED AT 13:40:40 ON 25 MAR 95)
L28 308 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23) FUL

FILE 'CA' ENTERED AT 14:05:18 ON 25 MAR 95
L29 75 S L28
L30 2 S L29(L) (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IMMU
L31 2 S L29 AND (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IM

FILE 'REGISTRY' ENTERED AT 14:07:02 ON 25 MAR 95

FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95

=> d all

L31 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS

AN 120:289504 CA

TI Highly potent and selective inhibition of human
immunodeficiency virus by the bicyclam derivative
JM3100

AU De Clerco, Erik; Yamamoto, Naohiko; Pauwels, Rudi; Balzarini, Jan;
Witvrouw, Myriam; De Vreese, Karen; Debyser, Zeger; Rosenwirth,
Brigitte; Peichl, Peter; et al.

CS Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain, B-3000, Belg.

SO Antimicrob. Agents Chemother. (1994), 38(4), 668-74

CODEN: AMACCQ; ISSN: 0066-4804

DT Journal

LA English

CC 1-5 (Pharmacology)

AB Bicyclams, in which the cyclam (1,4,8,11-tetraazacyclotetradecane)
moieties are tethered via an aliph. bridge (i.e., propylene, as in
JM2763) are potent and selective inhibitors of human
immunodeficiency virus type 1 (HIV-1)
and type-2 (HIV-2) (E. De Clercq, N. Yamamoto, R. Pauwels,
M. Baba, D. Schols, H. Nakashima, J. Balzarini, Z. Debyser, B. A.,
Murrer, D. Schwartz, D. Thornton, G. Bridger, S. Fricker, G. Henson,
M. Abrams, and D. Picker, Proc. Natl. Acad. Sci. USA 89:5286-5290,
1992). The authors have now found that the bicyclam JM3100, in
which the cyclam moieties are tethered by an arom. bridge [i.e.,
phenylenebis(methylene)], inhibits the replication of various
HIV-1 and HIV-2 strains in various cell lines at a
50% effective concn. (EC50) of 1 to 10 ng/mL, which is about
100-fold lower than the concn. required for JM2763 to inhibit
HIV replication and at least 100,000-fold lower than the
concn. required for JM2763 to inhibit HIV replication and
at least 100,000-fold lower than the cytotoxic concn. (>500
.mu.g/mL). In primary T4 lymphocytes or primary monocytes, JM3100
proved inhibitory to HIV-1 (IIIB) and several clin.

HIV-1 isolated at an EC50 of less than 1 ng/mL. On the
basis of time-of-addn. expts., JM3100 appeared to interact with a
viral uncoating event, and this was further corroborated by an
uncoating assay in which RNase sensitivity of [5-3H]uridine-labeled
virions was monitored. In addn., but possibly mechanistically
related, JM3100 blocks formation of infectious particles. JM3100
was also found to interfere directly with virus-induced
syncytium formation, albeit at a higher concn. (1 to 2 .mu.g/mL)
than that required for inhibition of viral replication. Following
s.c. injection of 10 mg of JM3100 per kg of body wt. to rabbits,
anti-HIV activity was detected in serum corresponding to
serum drug levels exceeding for at least 6 h by >100-fold the EC50
required to inhibit HIV replication in vitro. When
combined with either 3'-azido-2',3'-dideoxythymidine or
2',3'-dideoxyinosine, JM3100 achieved a additive inhibition of
HIV replication, and when repeatedly subcultivated in the
presence of JM3100, the virus remained insensitive to the
compd. for at least 30 passages (120 days) in cell culture.

ST HIV virus inhibition bicyclam deriv JM3100

IT Virucides and Virustats

(bicyclam derivs. as, structure in relation to, in human cells)

IT Drug interactions

(of bicyclam deriv. JM3100 and dideoxynucleosides, in HIV virus inhibition in human cells)

IT Drug resistance
(to bicyclam deriv. JM3100, in HIV virus in human cells)

IT Virus, animal
(human immunodeficiency 1, inhibition of, by bicyclam deriv. JM3100, in human cells)

IT Virus, animal
(human immunodeficiency 2, inhibition of, by bicyclam deriv. JM3100, in human cells)

IT Microbicidal and microbiostatic action
(virucidal, of bicyclam deriv. JM3100, against HIV virus in human cells)

IT Molecular structure-biological activity relationship
(virucidal, of bicyclam derivs., against HIV virus in human cells)

IT 30516-87-1, 3'-Azido-2',3'-dideoxythymidine 69655-05-6,
2',3'-Dideoxyinosine
(HIV virus inhibition by, bicyclam deriv. JM3100 enhancement of, in human cells)

IT 155148-31-5
(HIV virus inhibition by, mechanism of, structure in relation to, in human cells)

IT 110078-40-5, JM2763 110078-44-9 151191-06-9
151191-09-2 155148-32-6
(HIV virus inhibition by, structure in relation to, in human cells)

=> fil reg

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=> d 155148-31-5 110078-44-9

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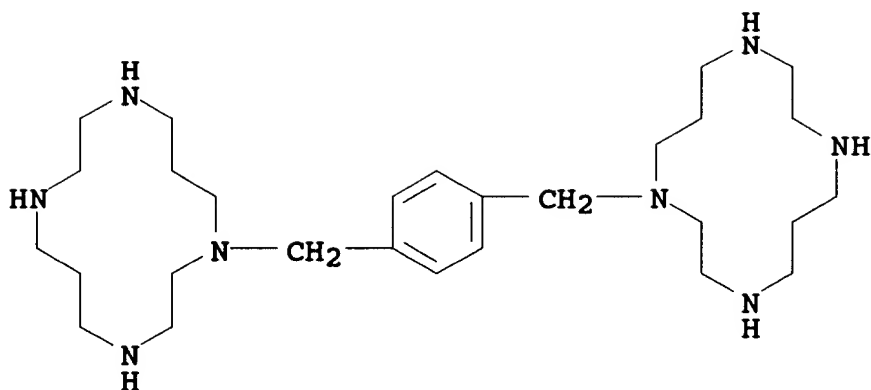
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)

MF C28 H54 N8 . 8 Cl H

SR CA

LC STN Files: CA, TOXLIT

CRN (110078-46-1)



*These compds
are in above*

● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 2 REGISTRY COPYRIGHT 1995 ACS

RN 110078-44-9 REGISTRY

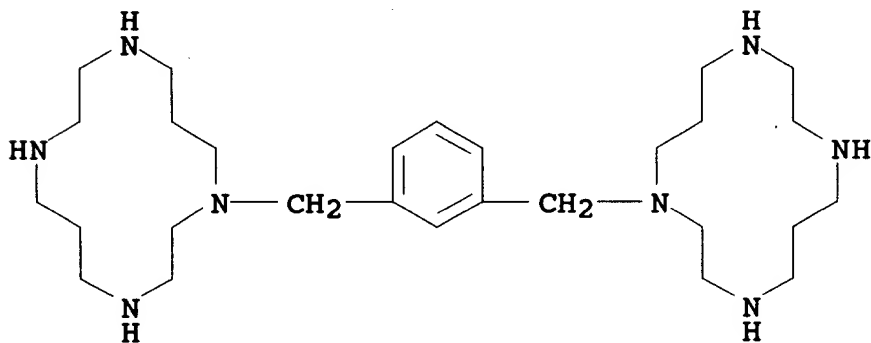
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C28 H54 N8

SR CA

LC STN Files: BEILSTEIN*, CA, CHEMINFORMRX, CJACS, TOXLIT, USPATFULL
(*File contains numerically searchable property data)



5 REFERENCES IN FILE CA (1967 TO DATE)

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L31 ANSWER 2 OF 2 CA COPYRIGHT 1995 ACS

AN 120:30786 CA

TI Linked heterocyclic polyamines with activity against HIV

IN Bridger, Gary James; Padmanabhan, Sreenivasan; Skerlj, Renato Tony;
Thornton, David Michael

PA Johnson Matthey P.L.C., UK

SO PCT Int. Appl., 66 pp.

CODEN: PIXXD2

PI WO 9312096 A1 930624

DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AI WO 92-GB2334 921216

PRAI GB 91-26677 911216

DT Patent

LA English

IC ICM C07D257-02

ICS C07D255-02; C07D259-00; C07D401-14; C07D409-14

CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

OS MARPAT 120:30786

AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 =
(un)substituted alk. chain or heteroatom-contg. chain; Y, Z = cyclic
polyamine moieties having 9-32 ring members and 3-8 N atoms in the
ring spaced by .gtoreq.2 C atoms from each other] or their acid
addn. salts or metal complexes are prepd. and demonstrated viricidal
activity against HIV-1 and HIV-2. Thus,
1,1'-[1,4-phenylenebis(methylene)]bis-1,4,8,11-
tetraazacyclotetradecane was prepd. and demonstrated 50% inhibitory
concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory
concn. against HIV-2 of <0.01 .mu.g/mL in an assay
employing infected MT-4 cells.

ST AIDS treatment prepn heterocyclic polyamine; HIV

virucide prepn heterocyclic polyamine;

tetraazacyclotetradecane prepn HIV viricidal agent;

virustat prepn tetraazacyclotetradecane

IT Virucides and Virustats

(heterocyclic polyamines)

IT Virus, animal

(human immunodeficiency 1, inhibition of, heterocyclic

polyamines for)
IT Virus, animal
(human immunodeficiency 2, inhibition of, heterocyclic
polyamines for)
IT 151191-32-1 151191-33-2 151191-34-3
151191-35-4 151191-36-5
(HIV viricidal activity of)
IT 7440-50-8DP, Copper, 1,4-phenylenebismethylene bis
tetraazacyclotetradecane complexes 7440-66-6DP, Zinc,
1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes
110078-44-9P 110078-46-1DP, copper and zinc
complexes 133587-10-7P 133587-11-8P
151190-72-6P 151190-73-7P 151190-74-8P
151190-75-9P 151190-76-0P 151190-80-6P
151190-81-7P 151190-85-1P 151190-87-3P
151190-91-9P 151190-93-1P 151190-94-2P
151190-95-3P 151190-96-4P 151190-97-5P
151190-98-6P 151190-99-7P 151191-02-5P
151191-03-6P 151191-05-8P 151191-06-9P
151191-08-1P 151191-09-2P 151191-12-7P
151191-14-9P 151191-15-0P 151191-17-2P
151191-18-3P 151191-20-7P 151191-21-8P
151191-24-1P 151191-25-2P 151191-26-3P
151191-27-4P 151191-28-5P 151191-29-6P
151191-30-9P 151191-31-0P 151191-37-6P
151191-38-7P 151191-39-8P
(prepn. and HIV viricidal activity of)
IT 19417-58-4P, 1,4-Benzenedipropanol 58791-49-4P 60023-32-7P
63134-93-0P 70364-29-3P 92339-07-6P 105355-16-6P
145617-64-7P 151190-69-1P 151190-70-4P
151190-71-5P 151190-77-1P 151190-79-3P 151190-82-8P
151190-83-9P 151190-84-0P 151190-86-2P 151190-88-4P
151190-89-5P 151190-92-0P 151191-00-3P
151191-01-4P 151191-04-7P 151191-07-0P
151191-10-5P 151191-11-6P 151191-13-8P
151191-16-1P 151191-19-4P 151191-22-9P
(prepn. and reaction of, in prepn. of heterocyclic HIV
viricidal agents)
IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-
Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3,
.alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2,
Carbethoxymethylene)triphenylphosphorane 1198-37-4,
2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane
7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4
39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1
104395-69-9 110078-46-1 134457-14-0 151190-78-2
151191-23-0
(reaction of, in prepn. of heterocyclic HIV viricidal
agents)

=> d 155148-31-5 110078-46-1 151191-07-0
'155148-31-5' IS NOT A VALID FORMAT FOR FILE 'CA'
'110078-46-1' IS NOT A VALID FORMAT FOR FILE 'CA'
'151191-07-0' IS NOT A VALID FORMAT FOR FILE 'CA'
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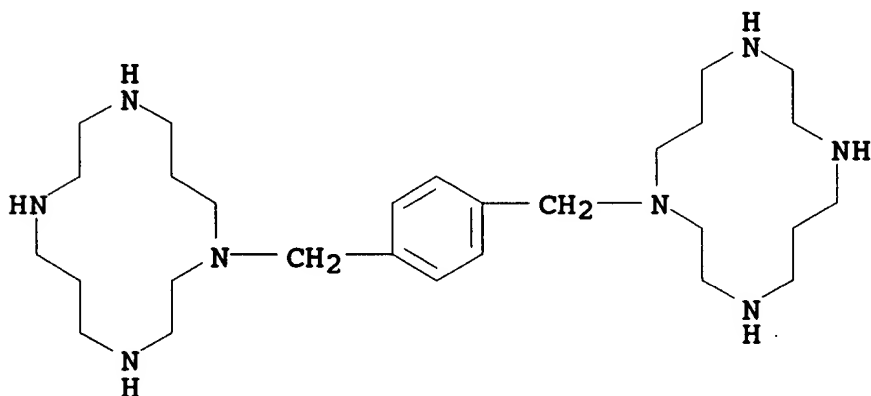
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-
phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX
NAME)

MF C28 H54 N8 . 8 Cl H

SR CA

LC STN Files: CA, TOXLIT

CRN (110078-46-1)



*These impols
are in above*

● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 2 REGISTRY COPYRIGHT 1995 ACS

RN 110078-46-1 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-
phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)

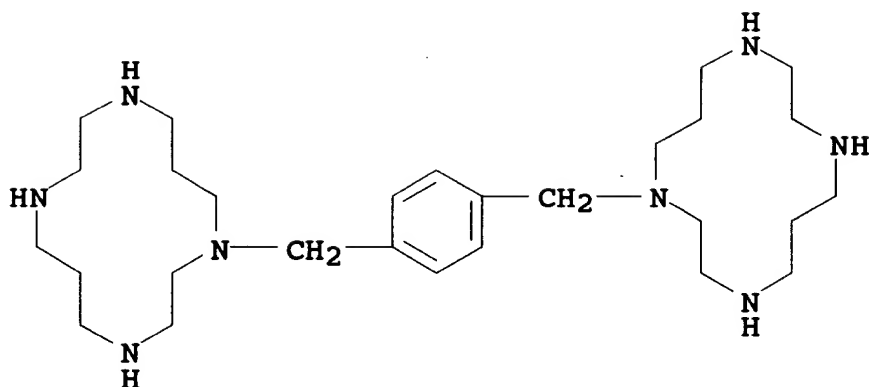
FS 3D CONCORD

MF C28 H54 N8

CI COM

SR CA

LC STN Files: BEILSTEIN*, CA, CJACS, USPATFULL
(*File contains numerically searchable property data)



4 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

ANSWER 3 REGISTRY COPYRIGHT 1995 ACS

RN 151191-07-0 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediylbis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)

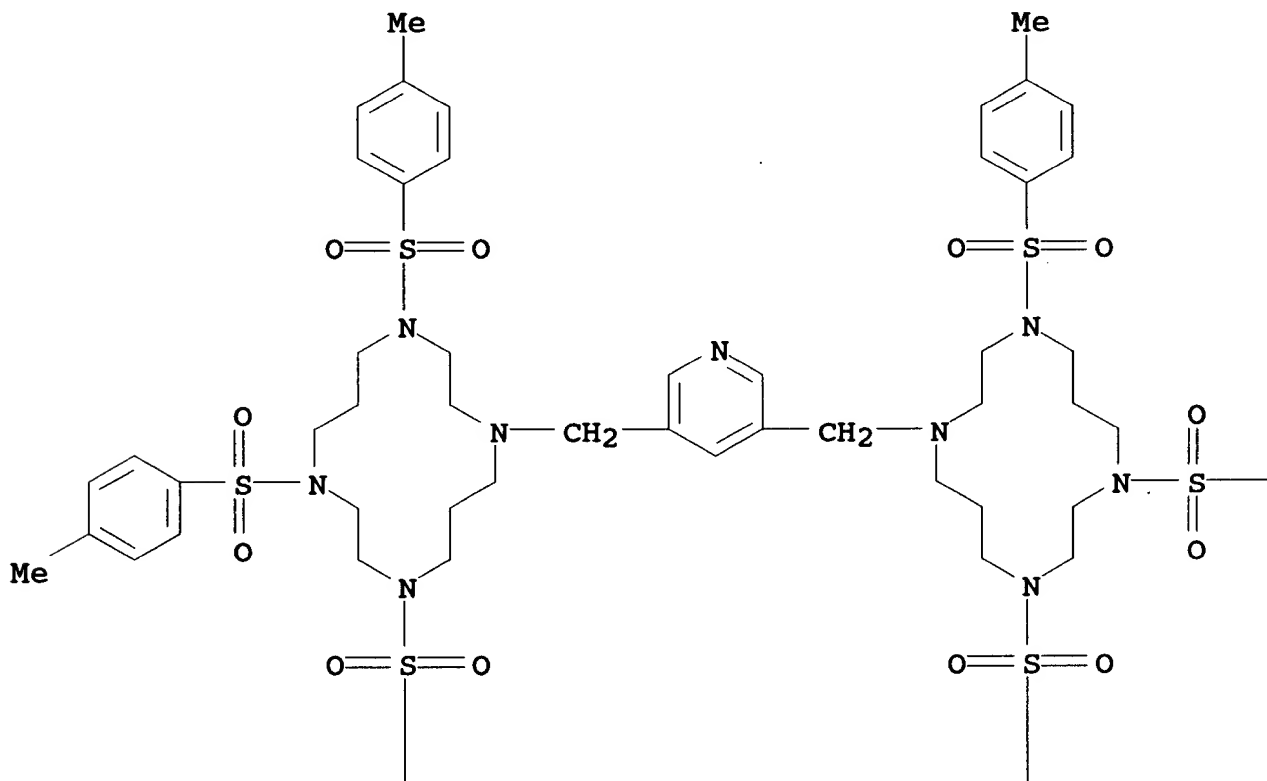
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MF C69 H89 N9 O12 S6

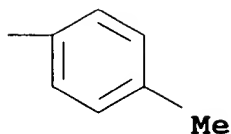
SR CA

LC STN Files: CA

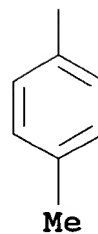
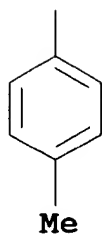
PAGE 1-A



PAGE 1-B



PAGE 2-A



1 REFERENCES IN FILE CA (1967 TO DATE)

=> d his

(FILE 'HOME' ENTERED AT 13:27:42 ON 25 MAR 95)

FILE 'REGISTRY' ENTERED AT 13:28:34 ON 25 MAR 95

L1 STR
L2 SCR 1847 AND 1996
L3 50 S L1 AND L2
L4 STR
L5 17 S L1 AND L4
L6 50 S L1 AND L4 AND L2

FILE 'CA' ENTERED AT 13:36:51 ON 25 MAR 95

L7 37 S BRIDGER G?/AU
L8 2 S L7 AND (HIV OR AIDS OR HTLV OR IMMUNODEFIC?)
L9 1 S L7 AND CYCLIC
L10 2 S L8 OR L9

FILE 'REGISTRY' ENTERED AT 13:39:08 ON 25 MAR 95

FILE 'REGISTRY' ENTERED AT 13:39:35 ON 25 MAR 95

FILE 'CA' ENTERED AT 13:40:04 ON 25 MAR 95

FILE 'REGISTRY' ENTERED AT 13:40:40 ON 25 MAR 95

L11 STR L1
L12 STR L4
L13 STR L12
L14 0 S L11 AND L12 AND L13
L15 SCR 1840 AND 1996
L16 4 S L11 AND L12 AND L13 AND L15
L17 STR L12
L18 3 S L11 AND L13 AND L17 AND L15
L19 STR
L20 4 S L11 AND L13 AND L17 AND L19 AND L15
L21 7 S L11 AND L13 AND L19 AND L15
L22 SCR 1840 AND 1996 AND 140 AND 1607 AND 1236
L23 SCR 1840 AND 1996 AND 140 AND 1607 AND 1363
L24 14 S L11 AND L13 AND L19 AND (L22 OR L23)
L25 8 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23)
L26 50 S L1 AND L13 AND L17 AND L19 AND (L22 OR L23)
L27 50 S L25 OR L26
L28 308 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23) FUL

FILE 'CA' ENTERED AT 14:05:18 ON 25 MAR 95

L29 75 S L28
L30 2 S L29(L) (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IMMU
L31 2 S L29 AND (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IM

FILE 'REGISTRY' ENTERED AT 14:07:02 ON 25 MAR 95

FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95

FILE 'REGISTRY' ENTERED AT 14:07:31 ON 25 MAR 95

FILE 'CA' ENTERED AT 14:08:05 ON 25 MAR 95

FILE 'REGISTRY' ENTERED AT 14:08:57 ON 25 MAR 95

FILE 'CA' ENTERED AT 14:09:21 ON 25 MAR 95

L32 4 S L29 AND PHARMAC?/SC,SX
L33 2 S L32 NOT L31

=>

=>

=> d all

L33 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS
AN 118:160633 CA
TI Synthesis, DNA binding interactions and biological activity of
bis-platinum (II) complexes of N,N,N',N'-tetrakis(2-
aminoethyl)diamines
AU Palmer, Brian D.; Wickham, Geoffrey; Craik, David J.; McFadyen, W.
David; Wakelin, Laurence P. G.; Baguley, Bruce C.; Denny, William A.
CS Sch. Med., Univ. Auckland, Auckland, N. Z.
SO Anti-Cancer Drug Des. (1992), 7(5), 385-401

CODEN: ACDDEA; ISSN: 0266-9536

- DT Journal
LA English
CC 1-6 (Pharmacology)
Section cross-reference(s): 23, 25, 78
- AB A series of dimers of the monofunctional platinum species [Pt(dien)Cl]⁺, linked by a variety of flexible (polymethylene) and more rigid chains, was prepd. and evaluated for DNA interactions and cytotoxic activity. The polymethylene-linked dimers were prepd. by acylation of N1,N3-bis(2-ethyl-2-imidazolidinyl)diethylenetriamine with .alpha.,.omega.-dicarboxylic acid chlorides, followed by redn. with diborane. Platination of these ligands was achieved with K₂PtI₄ prepd. in situ, followed by anion exchange. Solns. of the bis(Pt(dien)Cl)₂⁺ complexes were stable, and shown to be pure by ¹⁹⁵Pt NMR, but solid products could not be isolated. All of the bis(Pt(dien)Cl)₂⁺ complexes unwound closed circular supercoiled DNA more efficiently than the monomer, and were more efficient than the difunctional platinum complex cisplatin at crosslinking linearized plasmid DNA, as measured on non-denaturing agarose gels. None of the bis(Pt(dien)Cl)₂⁺ complexes were as cytotoxic as cisplatin in both the wild-type and platinum-resistant P388 murine leukemia cell lines. The more rigid analogs were equitoxic in both sensitive and cisplatin-resistant cells, but none showed in vitro activity against the P388 tumor.
- ST tetrakisaminoethyldiamine platinum complex antitumor prepn;
aminoethyldiamine platinum complex antitumor prepn
- IT Deoxyribonucleic acids
(bis-platinum tetrakis(aminoethyl)diamine complexes binding of, antitumor activity in relation to)
- IT Neoplasm inhibitors
(bis-platinum tetrakis(aminoethyl)diamine complexes, prepn. and DNA binding of)
- IT Crosslinking
(of bis-platinum tetrakis(aminoethyl)diamine complexes, by DNA)
- IT Kinetics, reaction
(of platinum tetrakis(aminoethyl)diamine complexes, with DNA, antitumor activity in relation to)
- IT 79-37-8, Oxalyl chloride 543-20-4, Succinyl chloride 1663-67-8, Malonyl chloride 90421-57-1
(acylation by, of bis(2-ethyl-2-imidazolidinyl)diethylenamine)
- IT 100-39-0, Benzyl bromide
(alkylation by, of bis(2-ethyl-2-imidazolidinyl)diethylenamine)
- IT 623-24-5 626-15-3 628-77-3, 1,5-Diiodopentane
(alkylation by, of bis(2-ethyl-2-imidazolidinyl)diethylenetriamine)
- IT 76-83-5, Trityl chloride
(alkylation by, of diethylenetriamine)
- IT 15663-27-1
(antitumor activity and DNA binding interaction of, aminoethyldiamine platinum complexes in relation to)
- IT 1877-77-6, 3-(Hydroxymethyl)aniline
(chlorine substitution reaction of)
- IT 10025-99-7
(complexation of, with diamines)
- IT 6232-88-8, 4-(Bromomethyl)benzoic acid
(conversion of, to acid chloride)
- IT 145901-58-2P
(prepn. and alkylation of, with benzyl halides or

haloalkylbenzamide derivs.)
IT 876-08-4P, 4-(Chloromethyl)benzoyl chloride
(prepn. and amidation by, of (chloromethyl)aniline)
IT 145883-50-7P
(prepn. and amidation of, with (chloromethyl)benzoyl chloride)
IT 14215-58-8P 18509-61-0P 145901-59-3P 146283-44-5P
146283-45-6P 146283-46-7P 146283-47-8P
146283-48-9P 146291-98-7P 146755-38-6P
(prepn. and antitumor activity of, DNA binding interaction in
relation to)
IT 145883-53-0P
(prepn. and complexation with platinum complexes)
IT 146735-46-8P
(prepn. and conversion to chloride complex)
IT 145883-52-9P 145883-54-1P 145883-59-6P
(prepn. and detritylation of)
IT 145883-51-8P
(prepn. and reaction with bistrityldiethylenetriamine)
IT 23539-10-8P 71277-15-1P 73571-38-7P 142745-41-3P
145883-55-2P 145883-61-0P 145883-62-1P
(prepn. and reaction with platinum complexes)
IT 145883-58-5P
(prepn. and redn. of)
IT 13528-04-6P 145883-56-3P 145883-57-4P 145883-60-9P
(prepn. of)
IT 111-40-0, Diethylenetriamine
(tritylation of)

=> fil reg;d 146283-46-7 146283-47-8 146291-98-7
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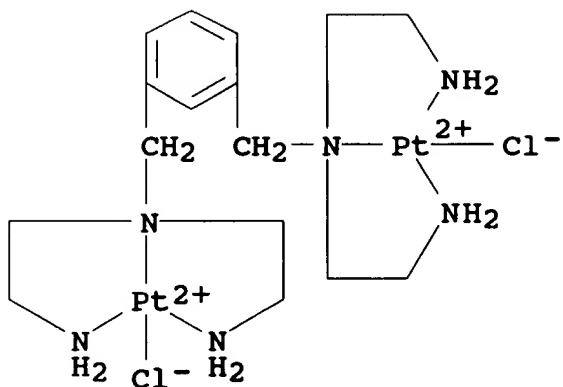
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RN 146283-46-7 REGISTRY
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1,3-
benzenedimethanamine-N1,N1',N1'':N3,N3',N3'']]di-, dichloride (9CI)
(CA INDEX NAME)
MF C16 H32 Cl2 N6 Pt2 . 2 Cl
CI CCS
SR CA
LC STN Files: CA, TOXLIT

*These compounds
are in
above*



● 2 Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 2 REGISTRY COPYRIGHT 1995 ACS

RN 146283-47-8 REGISTRY

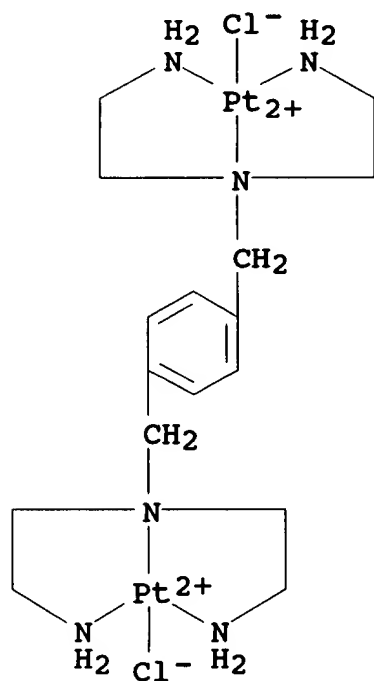
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1,4-benzenedimethanamine-N1,N1',N1'':N4,N4',N4'']]di-, dichloride (9CI)
(CA INDEX NAME)

MF C16 H32 Cl2 N6 Pt2 . 2 Cl

CI CCS

SR CA

LC STN Files: CA, TOXLIT



● 2 Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 3 REGISTRY COPYRIGHT 1995 ACS

RN 146291-98-7 REGISTRY

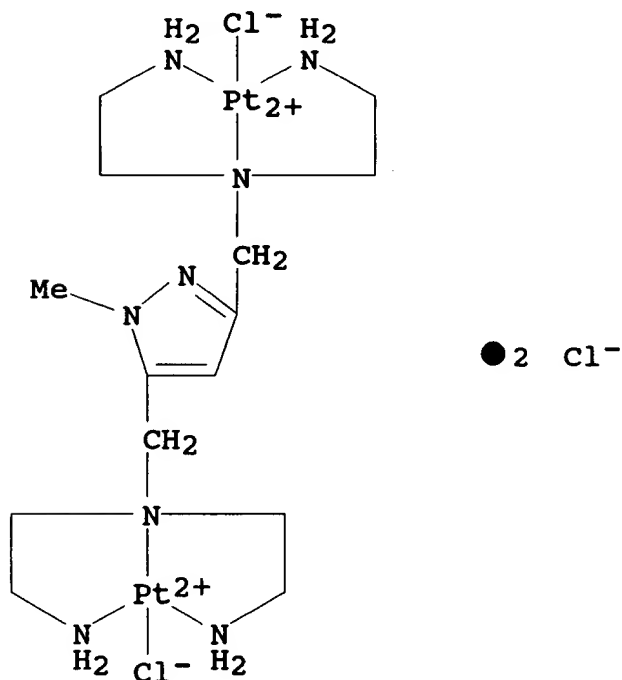
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1-methyl-1H-pyrazole-3,5-dimethanamine-N3,N3',N3':N5,N5',N5']]di-, dichloride (9CI) (CA INDEX NAME)

MF C14 H32 Cl2 N8 Pt2 . 2 Cl

CI CCS

SR CA

LC STN Files: CA, TOXLIT



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L33 ANSWER 2 OF 2 CA COPYRIGHT 1995 ACS

AN 97:119531 CA

TI Three-coordinate binuclear copper(I) complex: model compound for the copper sites in deoxyhemocyanin and deoxytyrosinase

AU Karlin, Kenneth D.; Gultneh, Yilma; Hutchinson, John P.; Zubieta, Jon

CS Cent. Biol. Macromol., State Univ. New York, Albany, NY, 12222, USA

SO J. Am. Chem. Soc. (1982), 104(19), 5240-2

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 1, 75

OS CJACS

AB The deoxy-binuclear Cu contg. active sites in the dioxygen carrier hemocyanin and the monooxygenase tyrosinase are through to contain 2 Cu(I) ions in close proximity which are each 2 or 3 coordinate and ligated to nitrogenous ligands. The synthesis and x-ray structural characterization of [Cu₂L](PF₆)₂ (I) (L = 1,3-[(RCH₂CH₂)₂NCH₂]₂C₆H₄, where = pyridyl) which mimics features of these deoxy sites is described. I contains a binucleating ligand where 2 tridentate groups with pyridyl and amino N-donors are connected by a m-xylyl connecting group. Each crystallog. independent Cu(I) ion is 3-coordinate in a similar distorted trigonal planar geometry with bonding parameters (av.); Cu-N(amino) = 2.16 .ANG.; Cu-N(pyridyl) = 1.92 .ANG.; N(amino)-Cu-N(pyridyl) = 99.8-104.3.degree. N(pyridyl)-Cu-N(pyridyl) = 150.9.degree.. The Cu(I) moieties are extended away from each other; Cu . . Cu = 8.940(2) .ANG.. I reacts with O in a manner analogous to the monooxygenases; it shows a quasireversible oxidn. wave at E_{1/2} = +0.16 V vs. NHE in DMF and reacts with CO and P-contg. ligands.

ST copper pyridylaminoxyl complex; crystal structure copper pyridylaminoxyl; xylyl pyridylamino copper complex

IT Crystal structure
Molecular structure

(of copper bis[bis(pyridylethyl)amino]-m-xylyl binuclear complex)

IT 82731-39-3P

(prepn. and crystal structure of)

IT 64443-05-6

(reaction of, with bis[bis(pyridylethyl)amino]-m-xylyl)

=> fil reg ;d 82731-39-3

FILE 'REGISTRY' ENTERED AT 14:11:13 ON 25 MAR 95

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

ANSWER 1 REGISTRY COPYRIGHT 1995 ACS

RN 82731-39-3 REGISTRY

CN Copper(2+), [μ -[N,N,N',N'-tetrakis[2-(2-pyridinyl)ethyl]-1,3-benzenedimethanamine-N1,N1',N1'':N3,N3',N3'']]di-,
bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,3-Benzenedimethanamine, N,N,N',N'-tetrakis[2-(2-pyridinyl)ethyl]-,
copper complex

CN Phosphate(1-), hexafluoro-, [μ -[N,N,N',N'-tetrakis[2-(2-pyridinyl)ethyl]-1,3-benzenedimethanamine-N1,N1',N1'':N3,N3',N3'']]dicopper(2+) (2:1)

MF C36 H40 Cu2 N6 . 2 F6 P

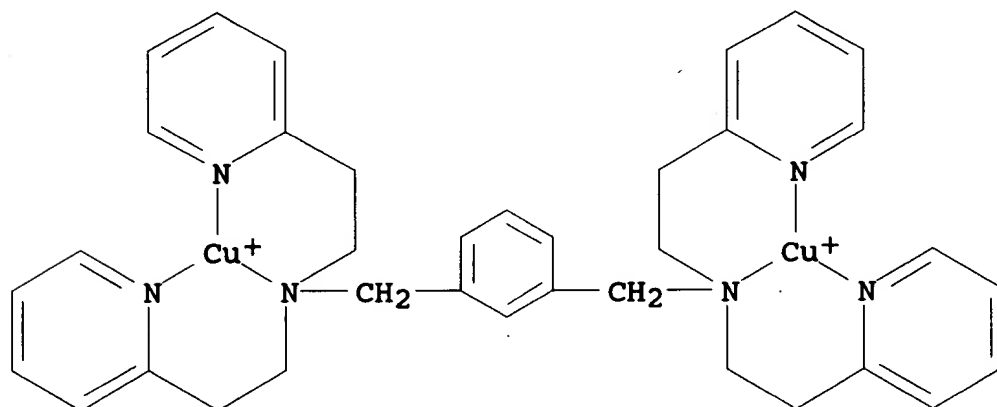
LC STN Files: CA, CJACS

CM 1

CRN 82281-84-3

CMF C36 H40 Cu2 N6

CCI CCS



*These compds are
in above cte*

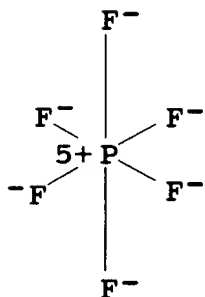
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CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



2 REFERENCES IN FILE CA (1967 TO DATE)

=> fil reg

FILE 'REGISTRY' ENTERED AT 14:27:59 ON 25 MAR 95
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STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

=> d que 140

L11 STR

N 1 N 3 N 5

NODE ATTRIBUTES:

NSPEC IS R AT 1

NSPEC IS R AT 3

NSPEC IS R AT 5

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L13 STR

N—C—Cy—C—N

1 2 3 4 5

NODE ATTRIBUTES:

NSPEC IS R AT 1

NSPEC IS R AT 5

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 3

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L17 STR

Hy—C—Cy—C—Hy

1 2 3 4 5

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS HIQ AT 1

GGCAT IS UNS AT 3

GGCAT IS HIQ AT 5

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M4 C M3 N AT 1

ECOUNT IS M4 C M3 N AT 5

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L19 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

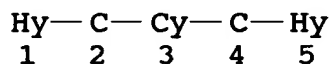
STEREO ATTRIBUTES: NONE

L22 SCR 1840 AND 1996 AND 140 AND 1607 AND 1236

L23 SCR 1840 AND 1996 AND 140 AND 1607 AND 1363

L28 308 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L17 AND L19 AND
(L22 OR L23)

L36 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS HIQ AT 1

GGCAT IS UNS AT 3

GGCAT IS HIQ AT 5

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M8 C E4 N AT 1

ECOUNT IS M8 C E4 N AT 5

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L40 137 SEA FILE=REGISTRY SUB=L28 SSS FUL L36

=> d his l41-

(FILE 'REGISTRY' ENTERED AT 14:11:13 ON 25 MAR 95)

L41 60 S L38 AND L40

L42 STR

L43 50 S L42

L44 111859 S 591.79.52/RID

L45 50 S L43 NOT L41

L46 57 S L41 NOT L44

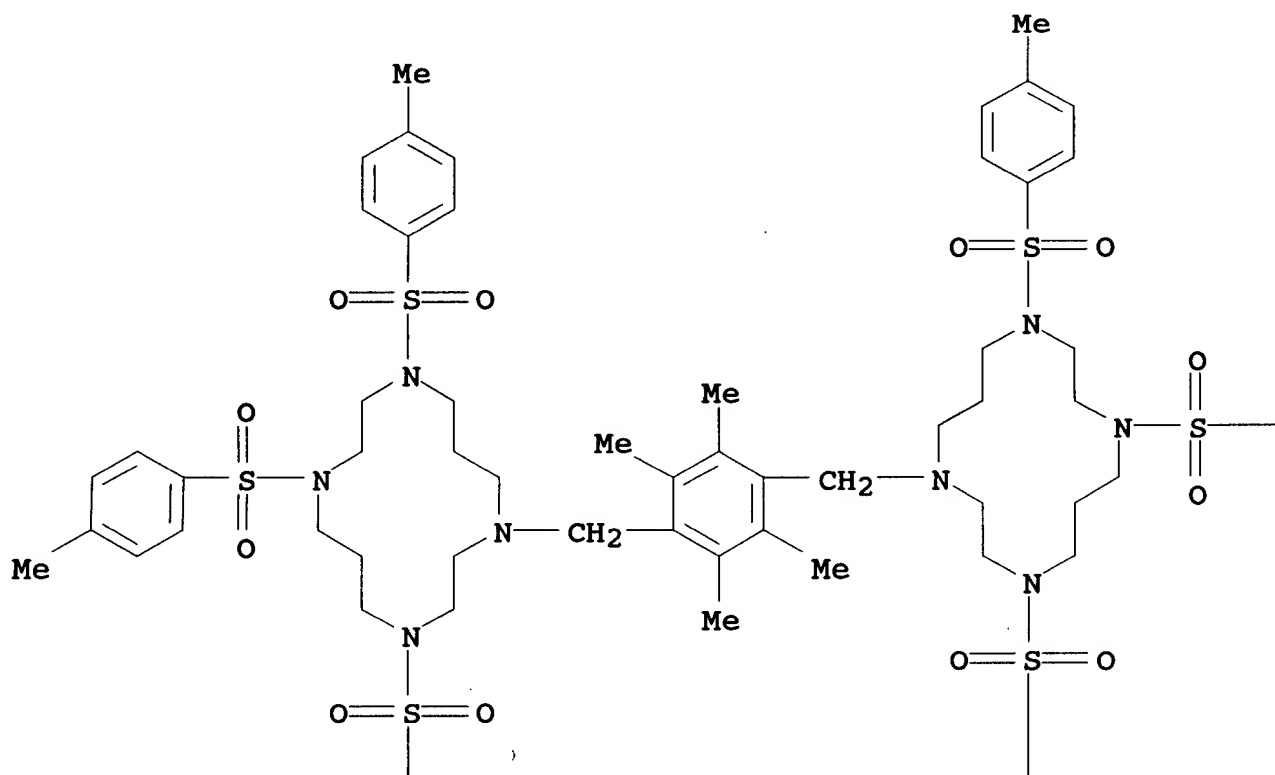
=> d 1-7 ide can

CN1CCN(CC1)CC2=C(C)C(C)=C(C)C2CC3CCNCCN3

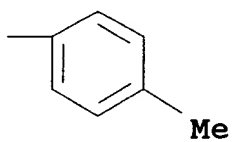
REFERENCE 1: 121:225706

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L46  ANSWER 2 OF 57  REGISTRY  COPYRIGHT 1995  ACS
RN   158200-25-0  REGISTRY
CN   1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,3,5,6-tetramethyl-1,4-
      phenylene)bis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]-
      (9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C74 H98 N8 O12 S6
SR   CA
LC   STN Files:    CA
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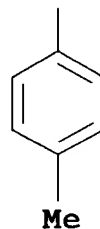
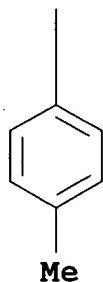
PAGE 1-A



PAGE 1-B



PAGE 2-A



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 121:225706

L46 ANSWER 3 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 155148-32-6 REGISTRY

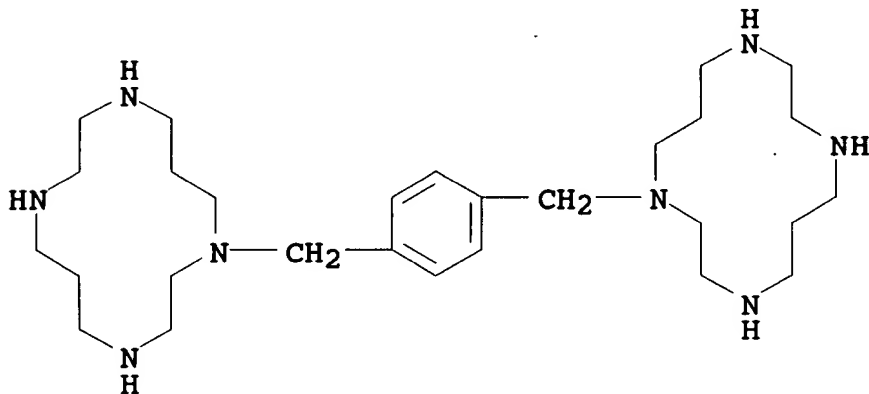
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrobromide (9CI) (CA INDEX NAME)

MF C28 H54 N8 . 8 Br H

SR CA

LC STN Files: CA, TOXLIT

CRN (110078-46-1)



● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

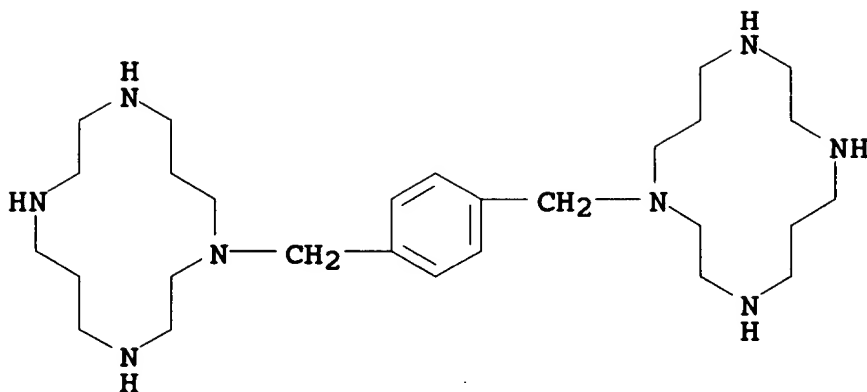
L46 ANSWER 4 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 155148-31-5 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)

MF C28 H54 N8 . 8 Cl H

SR CA
LC STN Files: CA, TOXLIT
CRN (110078-46-1)



● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

L46 ANSWER 5 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151987-13-2 REGISTRY

CN Cobalt(2+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']bis[carbonato(2-)-O,O']di-, dichloride, stereoisomer (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,4,7,10-Tetraazacyclododecane, cobalt(2+) deriv. (9CI)

MF C34 H50 Co2 N8 O6 . 2 Cl

CI CCS

SR CA

LC STN Files: CA

DES *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:44414

L46 ANSWER 6 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151956-64-8 REGISTRY

CN Cobalt(6+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']]tetraaquadi-, stereoisomer, hexanitrate (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,4,7,10-Tetraazacyclododecane, cobalt(6+) deriv. (9CI)

MF C32 H58 Co2 N8 O4 . 6 N O3

SR CA

LC STN Files: CA

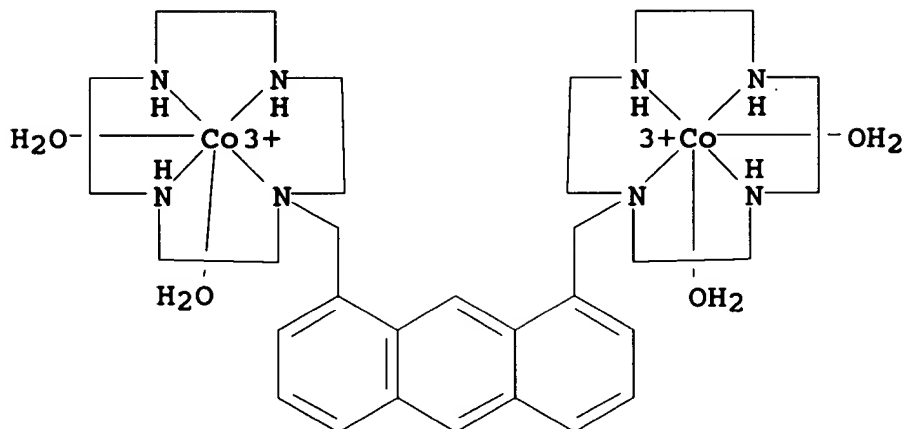
CM 1

CRN 151956-63-7

CMF C32 H58 Co2 N8 O4

CCI CCS

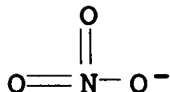
CDES *



CM 2

CRN 14797-55-8

CMF N O3



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:44414

L46 ANSWER 7 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151956-63-7 REGISTRY

CN Cobalt(6+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']]tetraaquadi-, stereoisomer (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

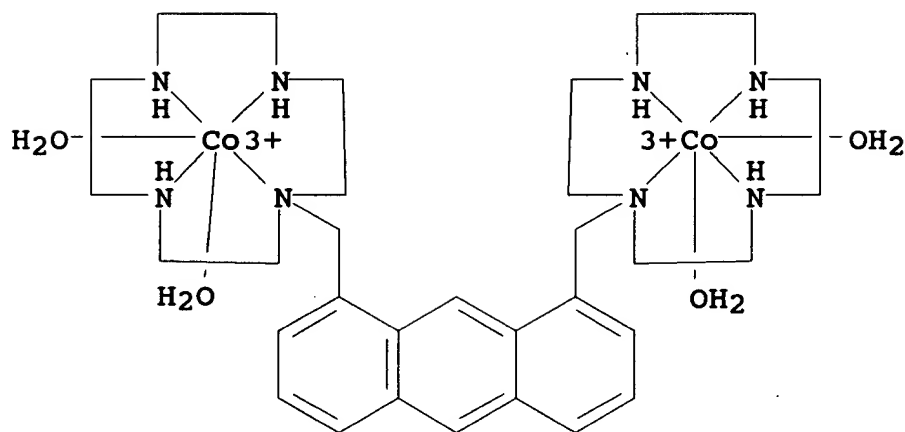
CN 1,4,7,10-Tetraazacyclododecane, cobalt(6+) deriv. (9CI)

MF C32 H58 Co2 N8 O4

CI CCS, COM

SR CA

DES *



=> d 8-30 ide can

L46 ANSWER 8 OF 57 REGISTRY COPYRIGHT 1995 ACS

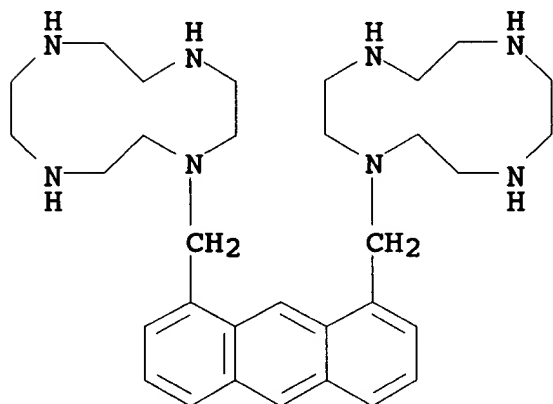
RN 151697-44-8 REGISTRY

CN 1,4,7,10-Tetraazacyclododecane, 1,1'-[1,8-anthracenediylbis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)

MF C32 H50 N8 . 8 Cl H

SR CA

LC STN Files: CA



● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

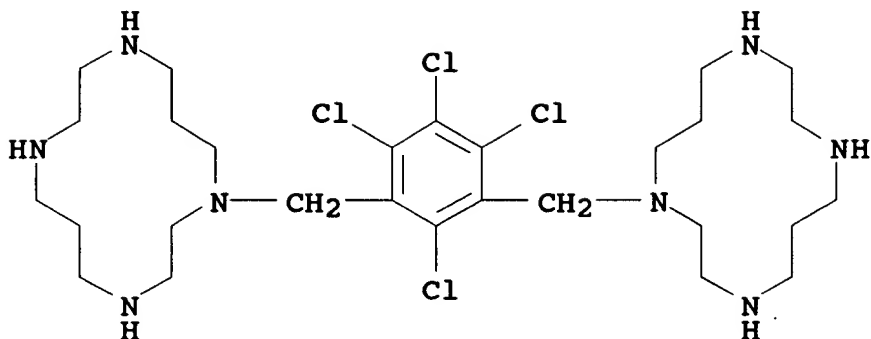
REFERENCE 1: 120:44414

L46 ANSWER 9 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-34-3 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,4,5,6-tetrachloro-1,3-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)

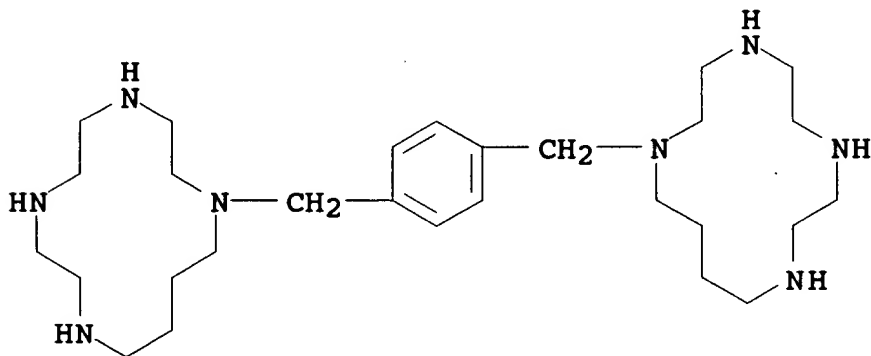
FS 3D CONCORD
MF C28 H50 Cl4 N8
CI COM
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 10 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-33-2 REGISTRY
CN 1,4,7,10-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8
SR CA
LC STN Files: CA

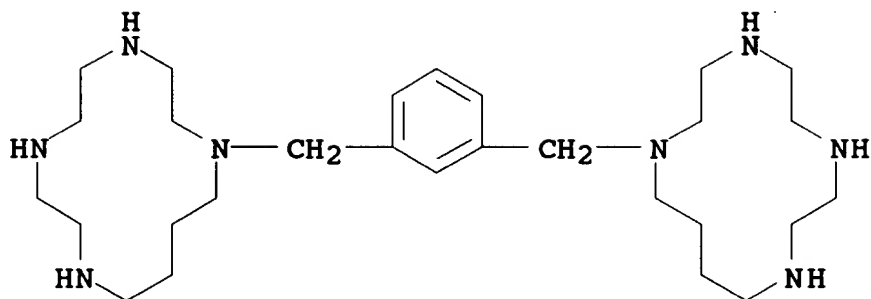


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 11 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-32-1 REGISTRY
CN 1,4,7,10-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8

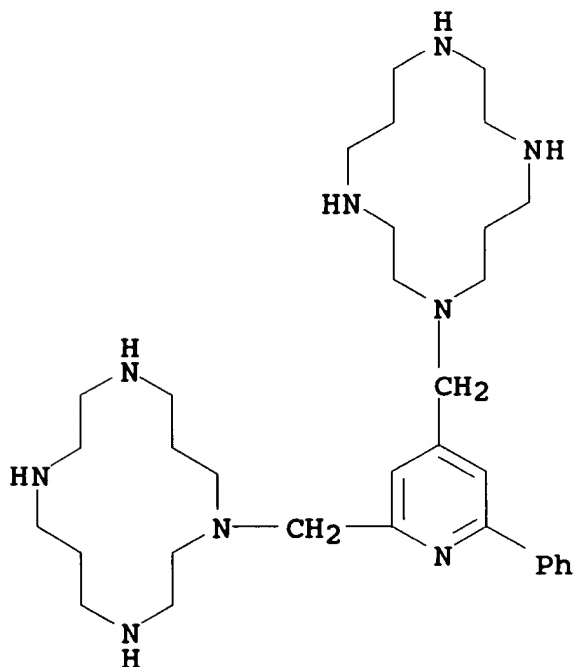
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

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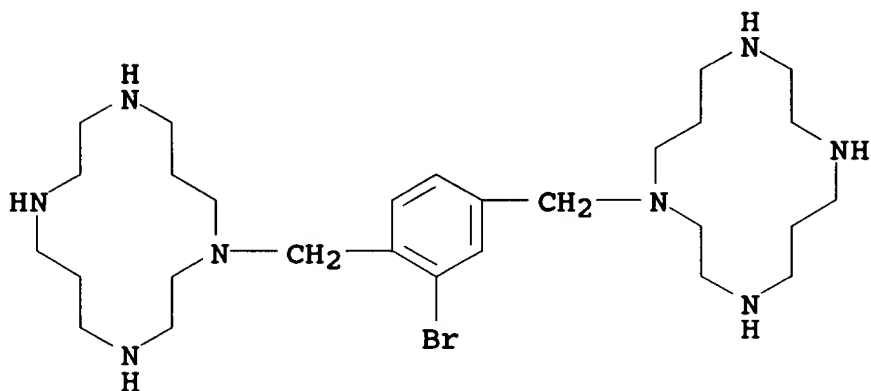
L46 ANSWER 12 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-31-0 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(6-phenyl-2,4-pyridinediyl)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C33 H57 N9
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

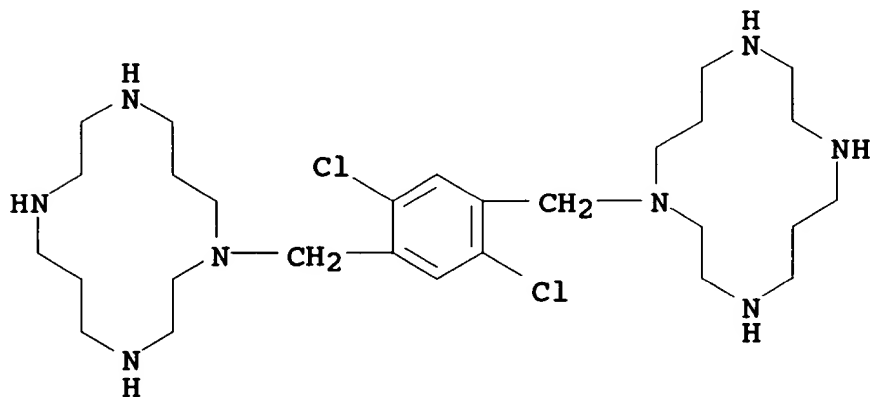
L46 ANSWER 13 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-30-9 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2-bromo-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H53 Br N8
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 14 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-29-6 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,5-dichloro-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H52 Cl2 N8
SR CA
LC STN Files: CA

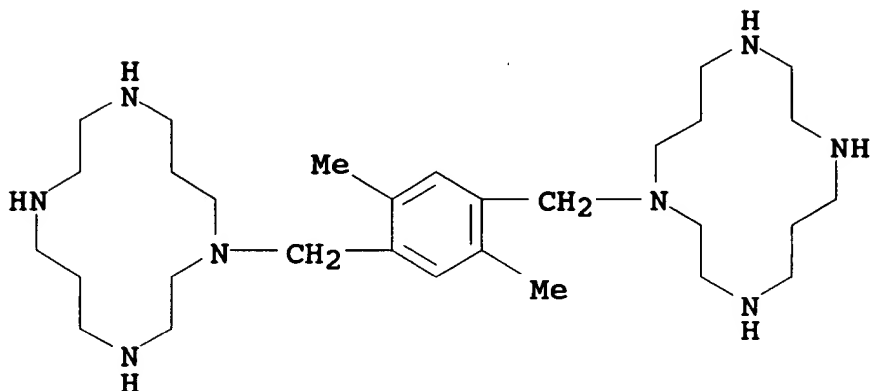


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 15 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-28-5 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,5-dimethyl-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)
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MF C30 H58 N8
SR CA
LC STN Files: CA

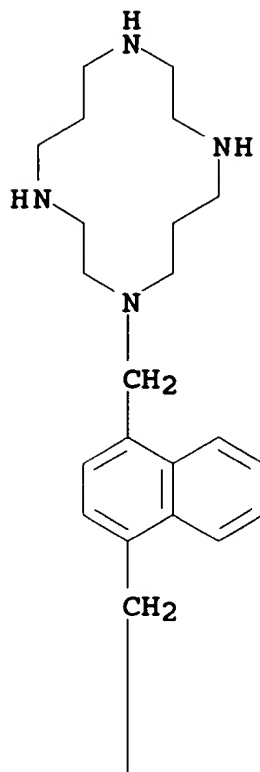


1 REFERENCES IN FILE CA (1967 TO DATE)

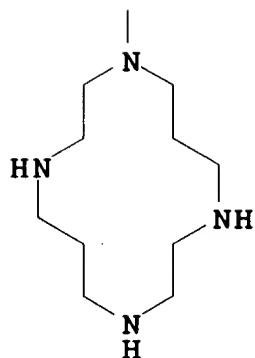
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L46 ANSWER 16 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-27-4 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-naphthalenediylbis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H56 N8
CI COM
SR CA
LC STN Files: CA

PAGE 1-A



PAGE 2-A



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 17 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-26-3 REGISTRY

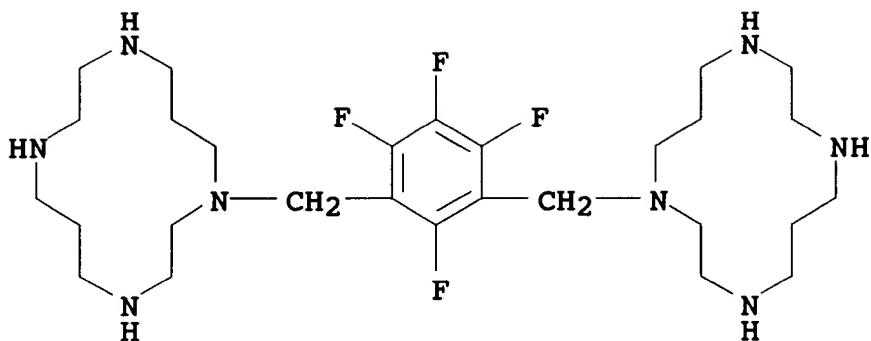
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,4,5,6-tetrafluoro-1,3-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C28 H50 F4 N8

SR CA

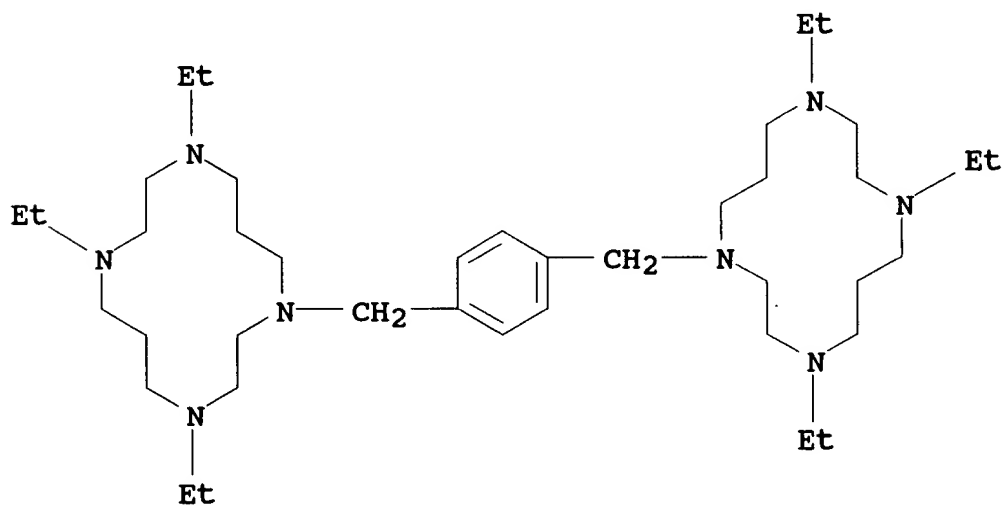
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 18 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-21-8 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C40 H78 N8
CI COM
SR CA
LC STN Files: CA

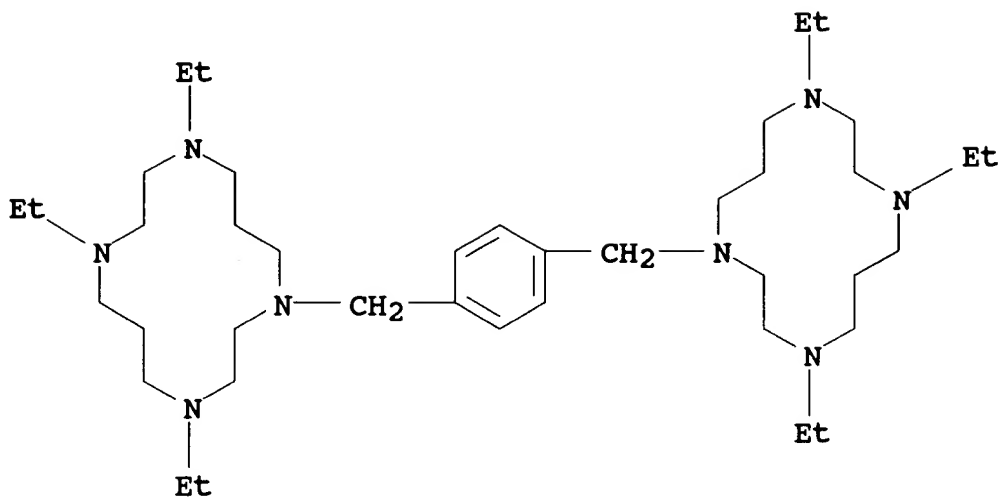


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 19 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-20-7 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triethyl-, octahydrobromide (9CI)

(CA INDEX NAME)
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SR CA
LC STN Files: CA
CRN (151191-21-8)

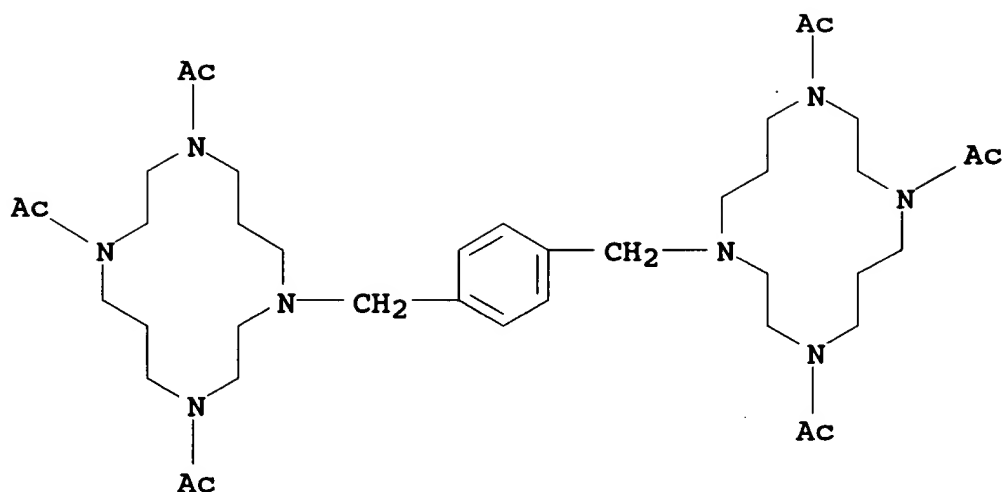


● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

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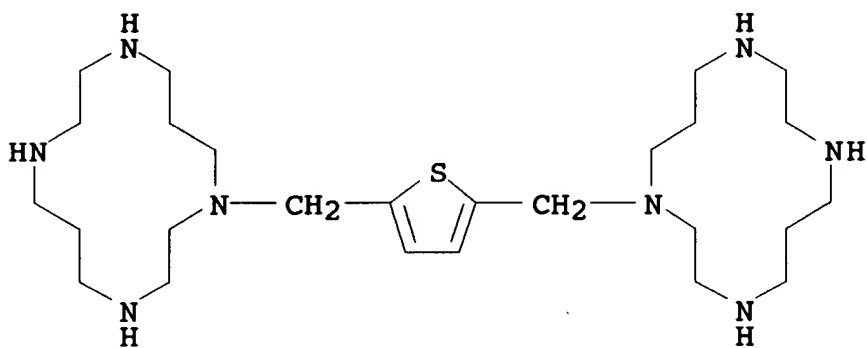
L46 ANSWER 20 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-19-4 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triacetyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C40 H66 N8 O6
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 21 OF 57 REGISTRY COPYRIGHT 1995 ACS
 RN 151191-18-3 REGISTRY
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,5-thiophenediylbis(methylene)]bis- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C26 H52 N8 S
 CI COM
 SR CA
 LC STN Files: CA

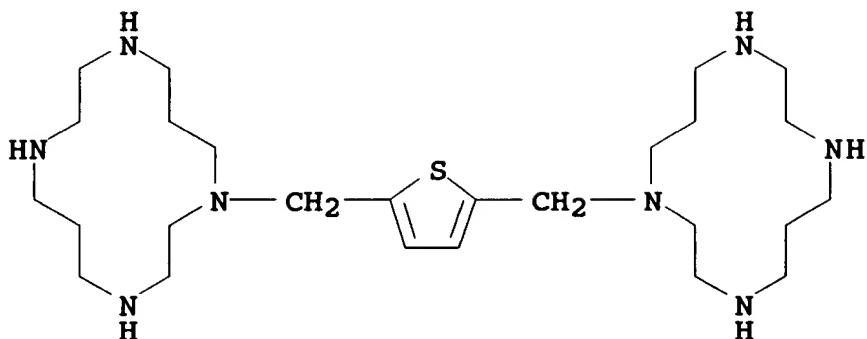


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 22 OF 57 REGISTRY COPYRIGHT 1995 ACS
 RN 151191-17-2 REGISTRY
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,5-thiophenediylbis(methylene)]bis-, octahydrobromide (9CI) (CA INDEX NAME)
 MF C26 H52 N8 S . 8 Br H

SR CA
LC STN Files: CA
CRN (151191-18-3)



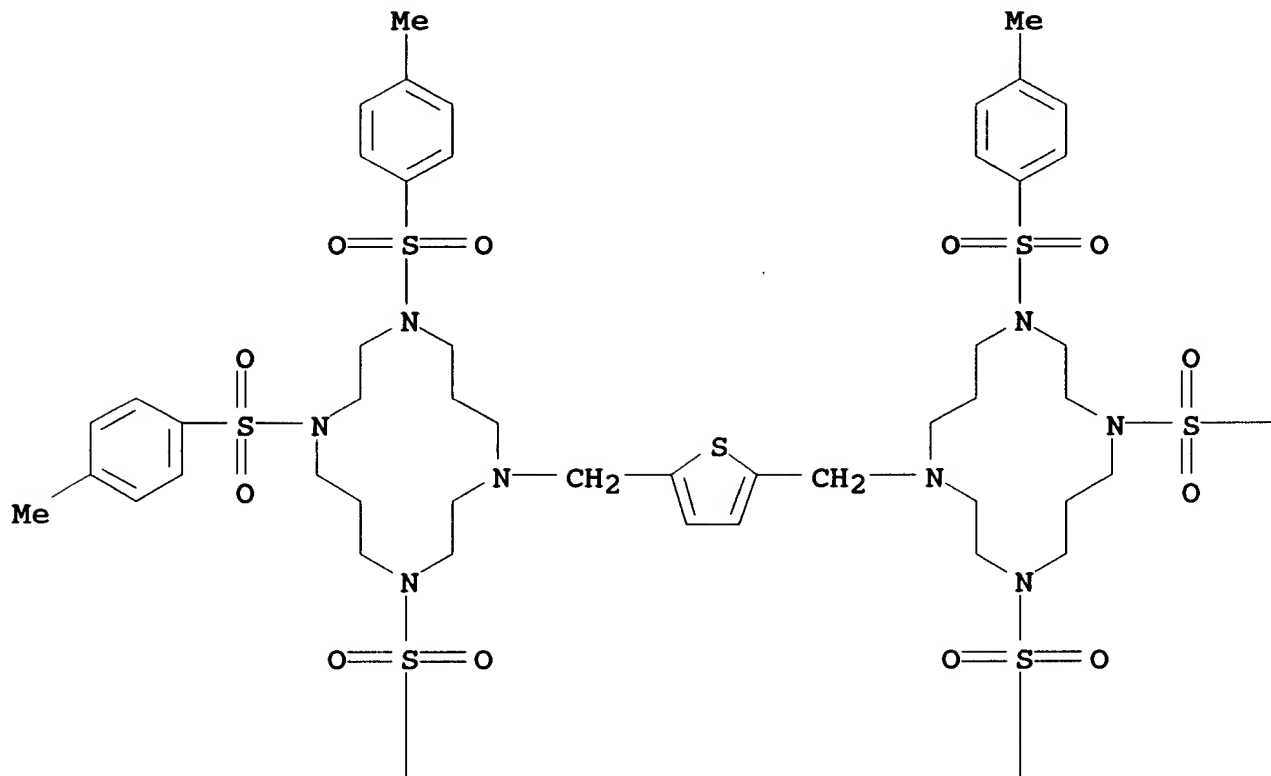
● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

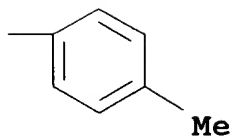
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L46  ANSWER 23 OF 57  REGISTRY  COPYRIGHT 1995 ACS
RN   151191-16-1  REGISTRY
CN   1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,5-
      thiophenediylbis(methylene)]bis[4,8,11-tris[(4-
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FS   3D CONCORD
MF   C68 H88 N8 O12 S7
SR   CA
LC   STN Files:    CA
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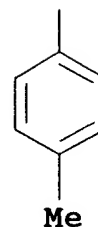
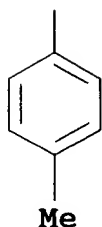
PAGE 1-A



PAGE 1-B



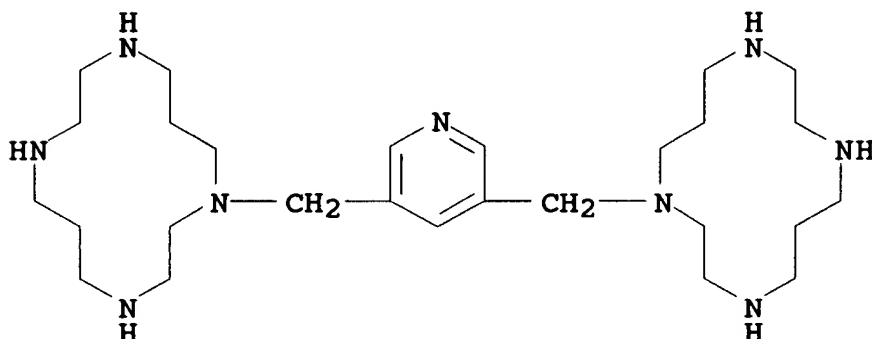
PAGE 2-A



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 24 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-09-2 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-
pyridinediylbis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H53 N9
CI COM
SR CA
LC STN Files: CA, TOXLIT

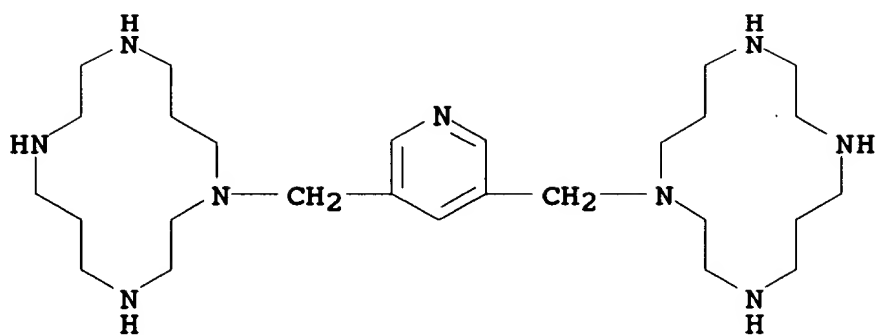


2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

REFERENCE 2: P 120:30786

L46 ANSWER 25 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-08-1 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-
pyridinediylbis(methylene)]bis-, nonahydrobromide (9CI) (CA INDEX
NAME)
MF C27 H53 N9 . 9 Br H
SR CA
LC STN Files: CA
CRN (151191-09-2)



● 9 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 26 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-07-0 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediylbis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)

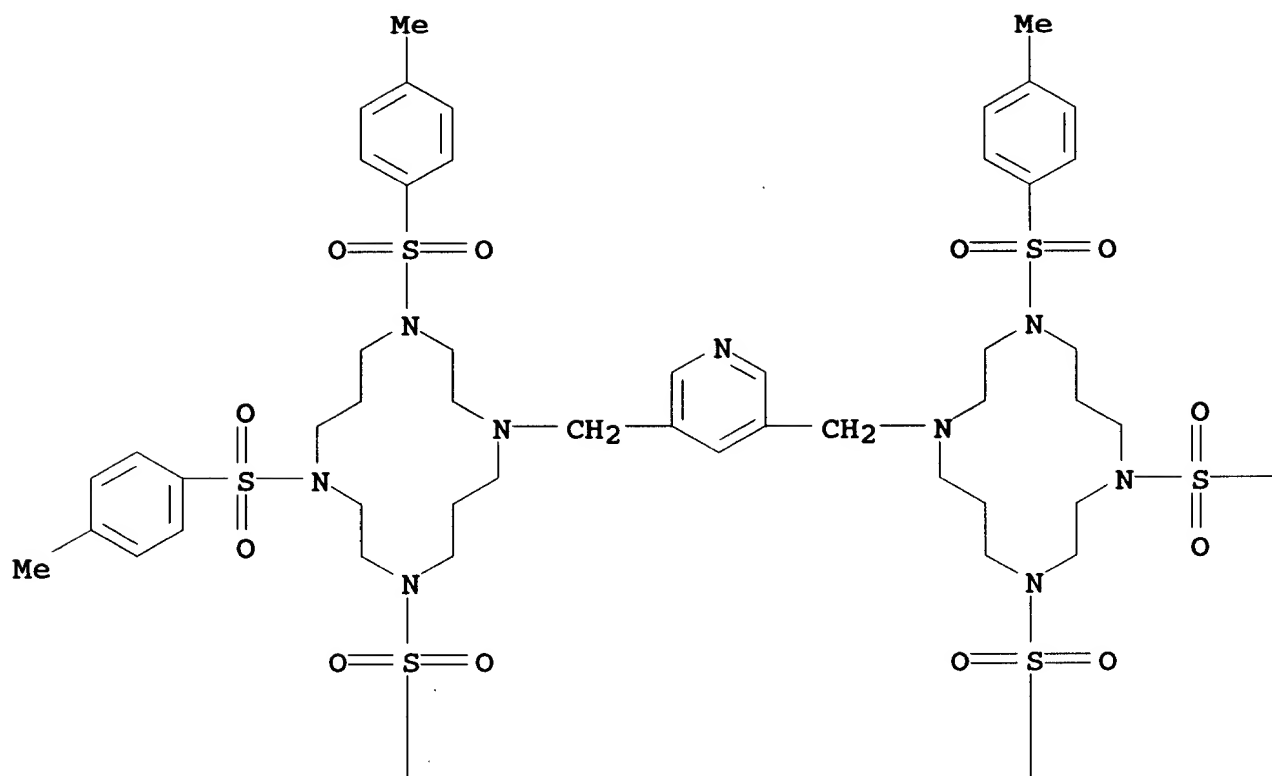
FS 3D CONCORD

MF C69 H89 N9 O12 S6

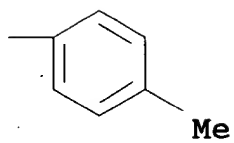
SR CA

LC STN Files: CA

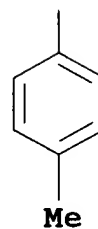
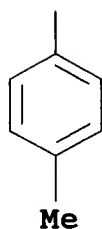
PAGE 1-A



PAGE 1-B



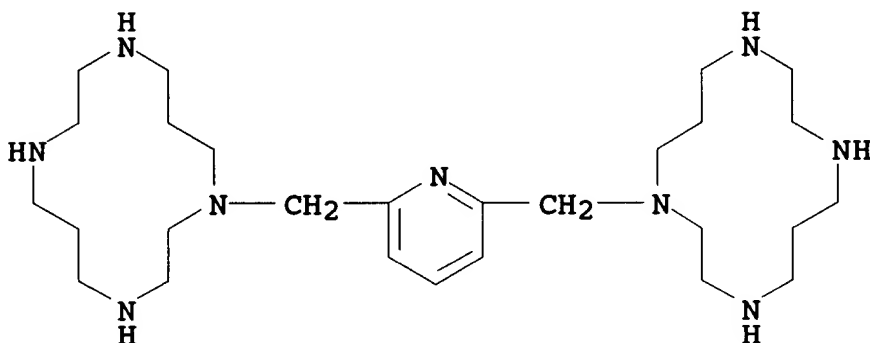
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1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 27 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-06-9 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,6-
pyridinediylbis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H53 N9
CI COM
SR CA
LC STN Files: CA, TOXLIT

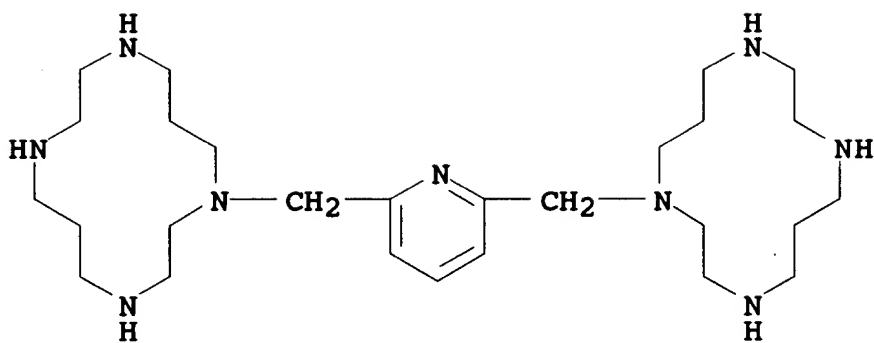


2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

REFERENCE 2: P 120:30786

L46 ANSWER 28 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-05-8 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,6-
pyridinediylbis(methylene)]bis-, octahydrobromide (9CI) (CA INDEX
NAME)
MF C27 H53 N9 . 8 Br H
SR CA
LC STN Files: CA
CRN (151191-06-9)



● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 29 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-04-7 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,6-pyridinediylbis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)

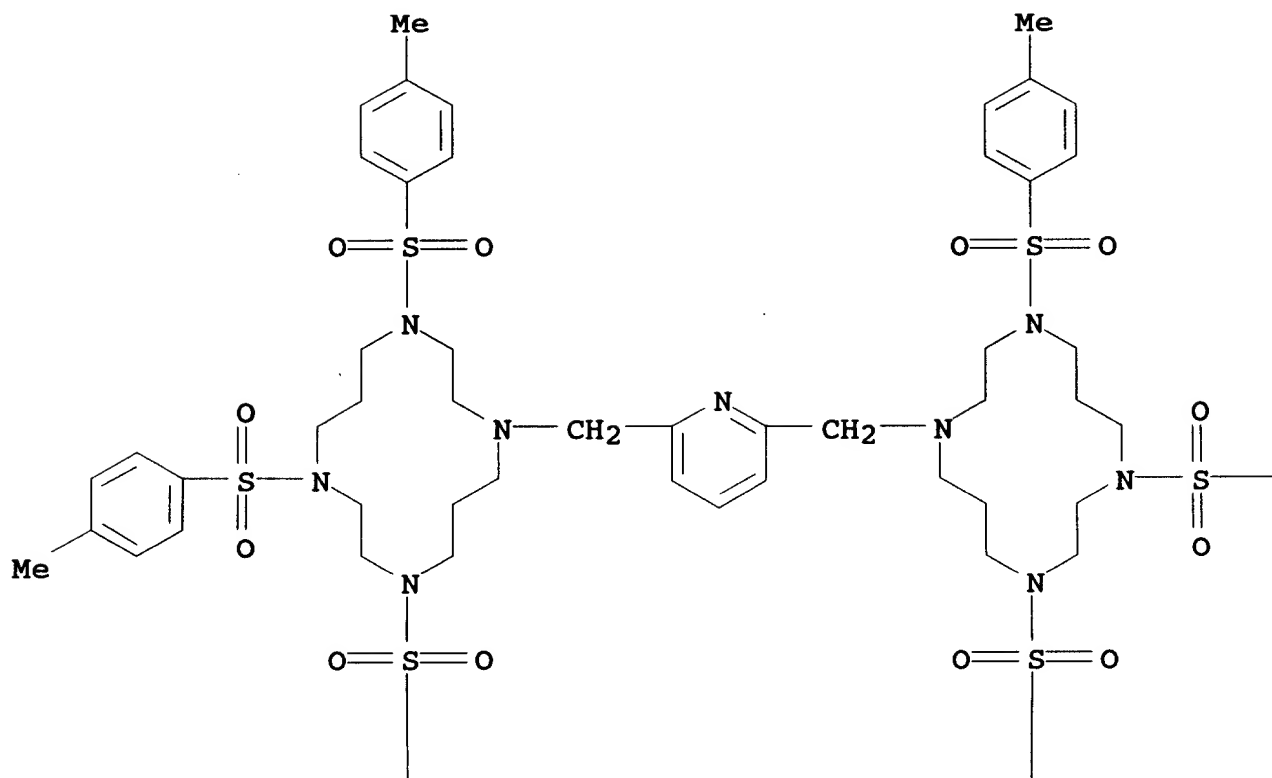
FS 3D CONCORD

MF C69 H89 N9 012 S6

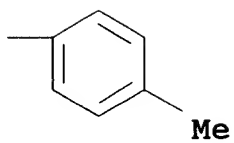
SR CA

LC STN Files: CA

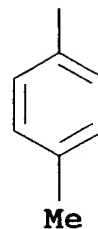
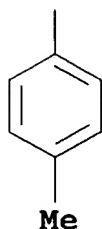
PAGE 1-A



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PAGE 2-A



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 30 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-03-6 REGISTRY

CN 1,4,7,11-Tetraazacyclotetradecane, 11-[[4-(1,4,8,11-tetraazacyclotetradec-1-ylmethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,4,8,11-Tetraazacyclotetradecane, 1,4,7,11-tetraazacyclotetradecane deriv. (9CI)

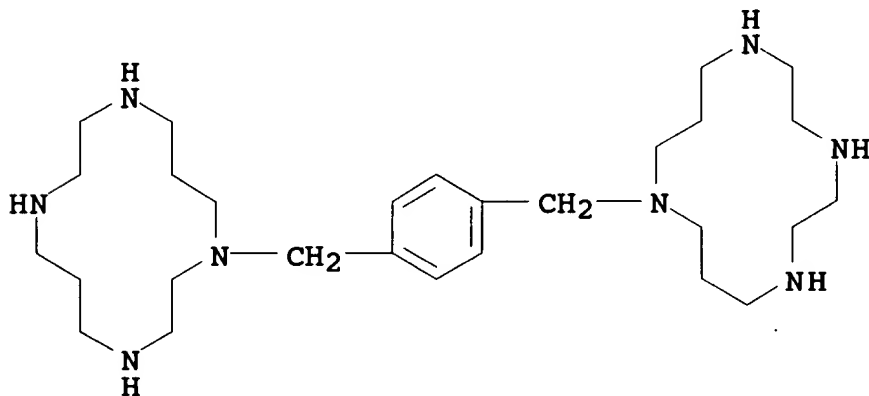
FS 3D CONCORD

MF C28 H54 N8

CI COM

SR CA

LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

=> d ide can 50-57

L46 ANSWER 50 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 142079-95-6 REGISTRY

CN Iron(2+), tris[1-([2,2'-bipyridin]-5-ylmethyl)-1,4,8,11-tetraazacyclotetradecane]-, (OC-6-21)- (9CI) (CA INDEX NAME)

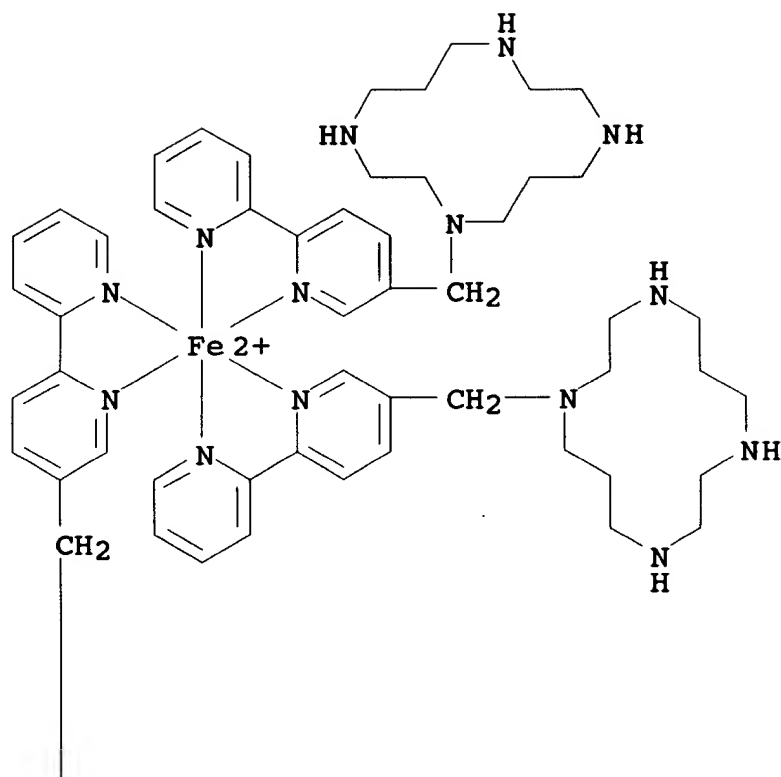
OTHER CA INDEX NAMES:

CN 1,4,8,11-Tetraazacyclotetradecane, iron(2+) deriv. (9CI)

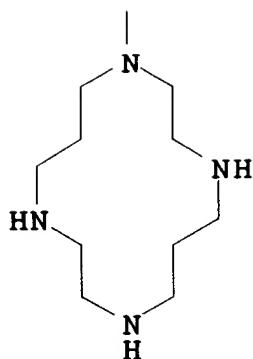
MF C63 H96 Fe N18

CI CCS
SR CA
LC STN Files: CA
DES 7:OC-6-21

PAGE 1-A



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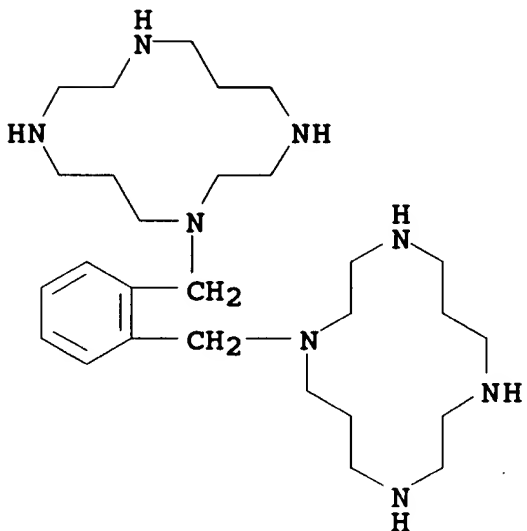


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 117:82274

L46 ANSWER 51 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 133563-60-7 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,2-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8
SR CA
LC STN Files: CA, USPATFULL

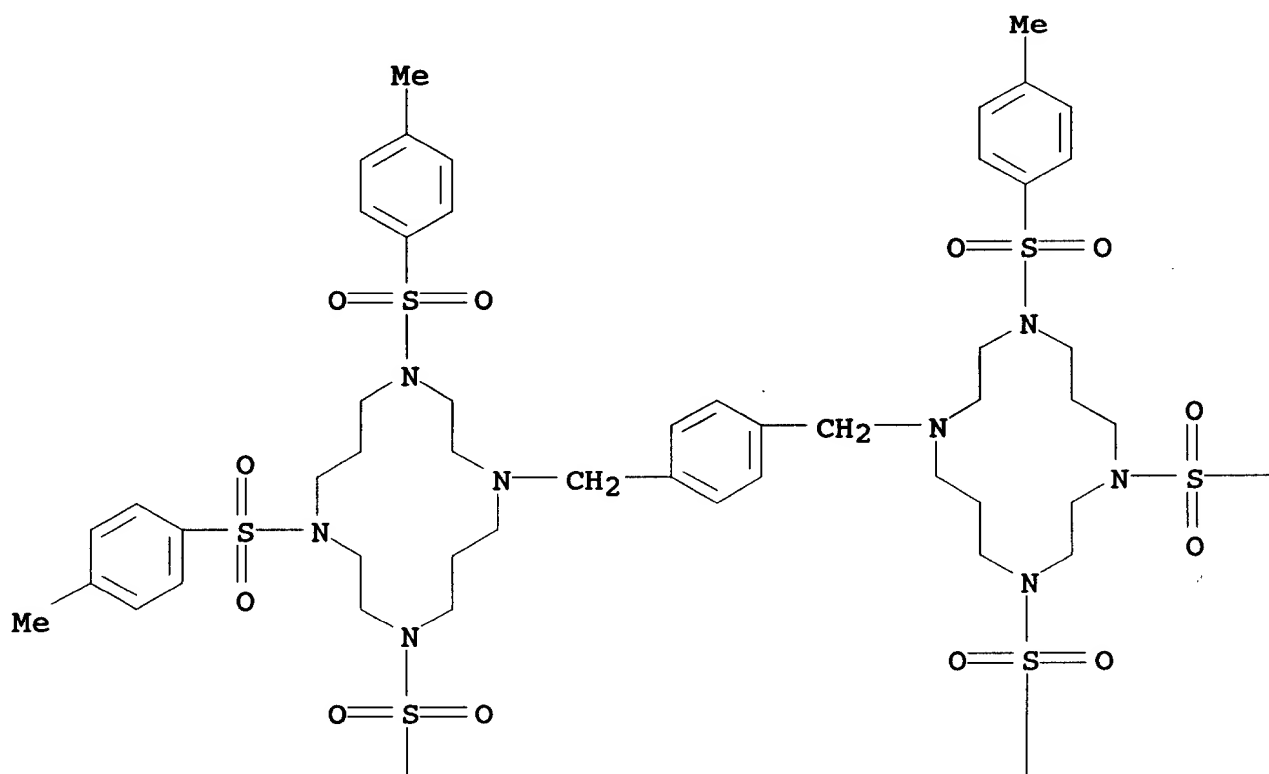


1 REFERENCES IN FILE CA (1967 TO DATE)

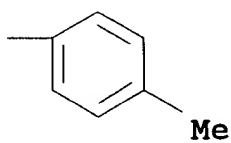
REFERENCE 1: P 114:207294

L46 ANSWER 52 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 110078-47-2 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C70 H90 N8 O12 S6
SR CA
LC STN Files: CA, CJACS

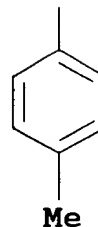
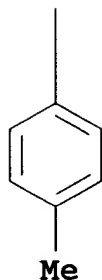
PAGE 1-A



PAGE 1-B



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1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 107:167695

L46 ANSWER 53 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 110078-46-1 REGISTRY

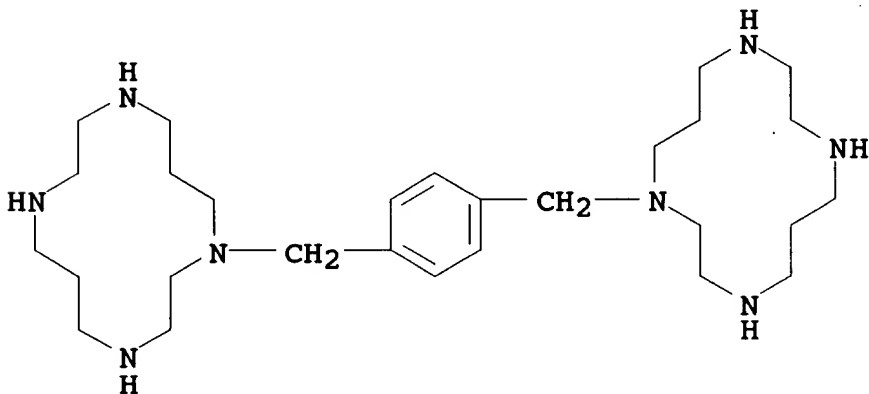
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C28 H54 N8

CI COM

SR CA

LC STN Files: BEILSTEIN*, CA, CJACS, USPATFULL
(*File contains numerically searchable property data)

4 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

REFERENCE 1: P 120:30786

REFERENCE 2: 118:204007

REFERENCE 3: P 114:207294

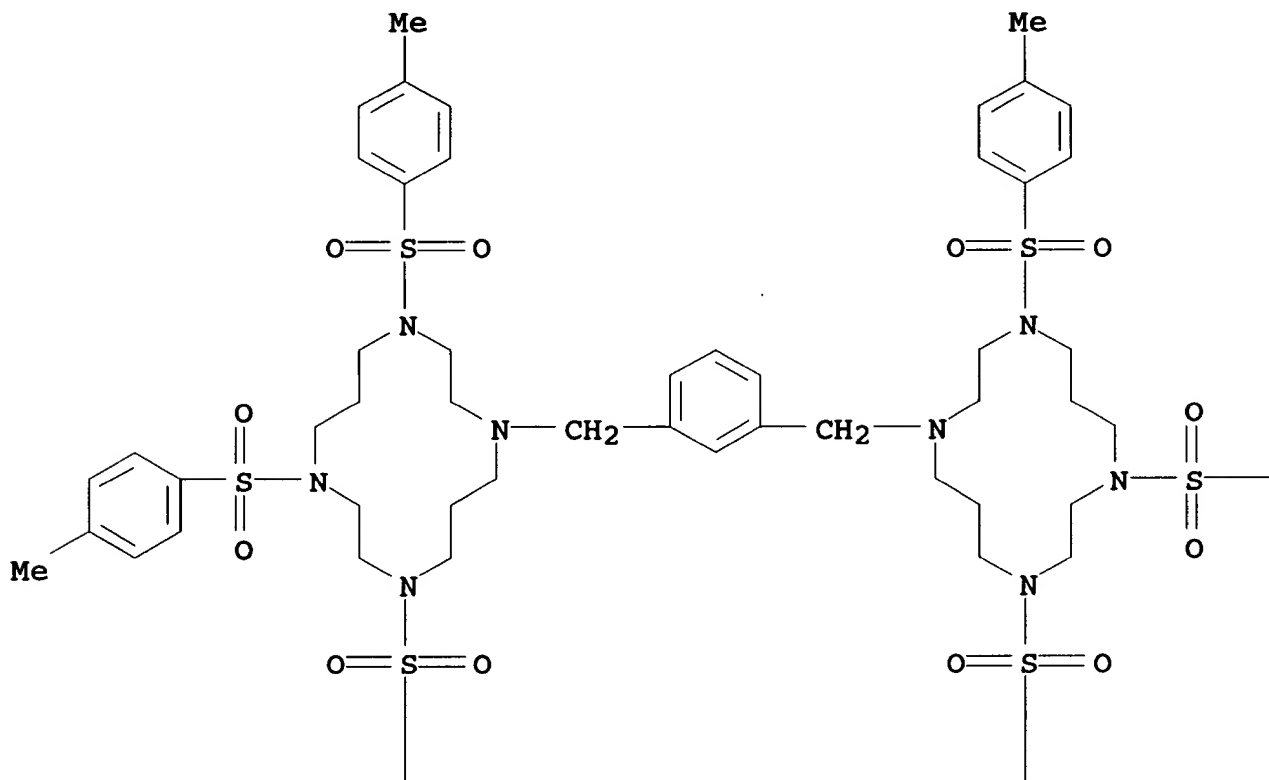
REFERENCE 4: 114:207229

REFERENCE 5: 107:167695

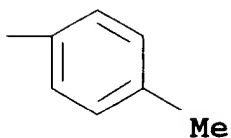
L46 ANSWER 54 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 110078-45-0 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C70 H90 N8 O12 S6
SR CA
LC STN Files: CA, CJACS

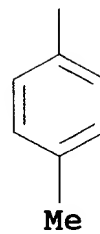
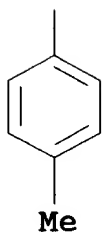
PAGE 1-A



PAGE 1-B



PAGE 2-A



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 107:167695

L46 ANSWER 55 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 110078-44-9 REGISTRY

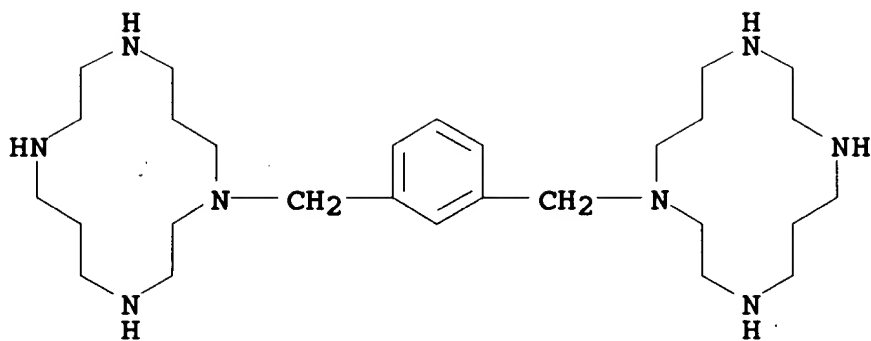
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C28 H54 N8

SR CA

LC STN Files: BEILSTEIN*, CA, CHEMINFORMRX, CJACS, TOXLIT, USPATFULL
(*File contains numerically searchable property data)



5 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

REFERENCE 2: P 120:30786

REFERENCE 3: P 114:207294

REFERENCE 4: 114:207229

REFERENCE 5: 107:167695

L46 ANSWER 56 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 105390-46-3 REGISTRY

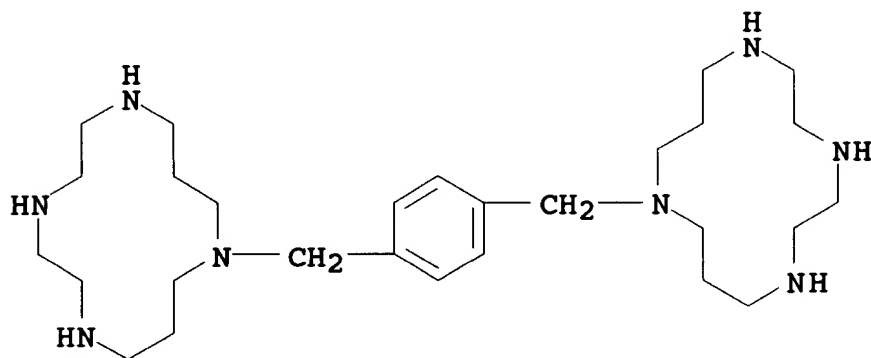
CN 1,4,7,11-Tetraazacyclotetradecane, 11,11'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)

MF C28 H54 N8 . 8 Cl H

SR CA

LC STN Files: CA

CRN (151190-99-7)



● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 106:26833

L46 ANSWER 57 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 105355-16-6 REGISTRY

CN 1,4,7,11-Tetraazacyclotetradecane, 11,11'-[1,4-phenylenebis(methylene)]bis[1,4,7-tris[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)

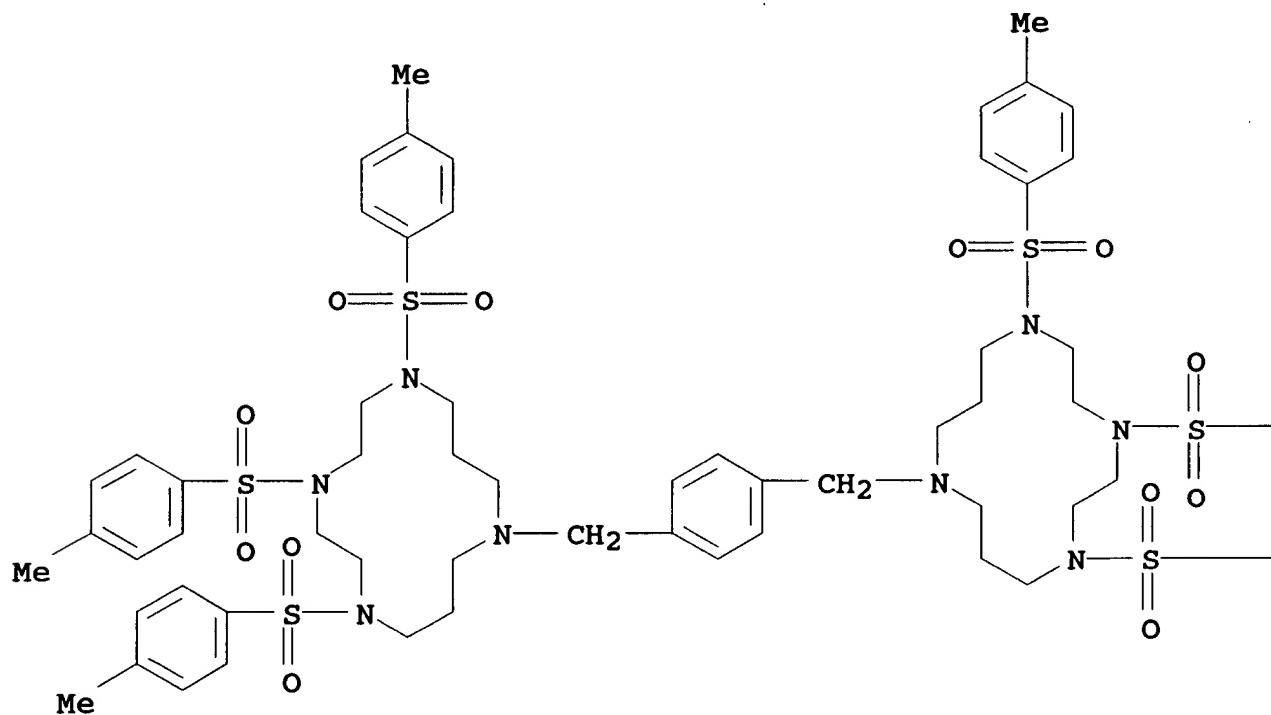
FS 3D CONCORD

MF C70 H90 N8 O12 S6

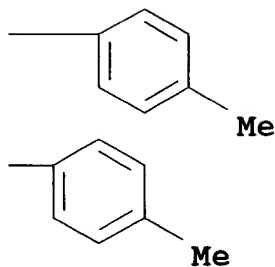
SR CA

LC STN Files: CA

PAGE 1-A



PAGE 1-B



2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

REFERENCE 2: 106:26833

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L47 10 L46

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L47 ANSWER 1 OF 10 CA COPYRIGHT 1995 ACS

AN 121:225706 CA

TI Synthetic Bis-Metal Ion Receptors for Bis-Imidazole "Protein
Analogues"

AU Mallik, Sanku; Johnson, Robert D.; Arnold, Frances H.

CS Division of Chemistry and Chemical Engineering 210-41, California
Institute of Technology, Pasadena, CA, 91125, USA

SO J. Am. Chem. Soc. (1994), 116(20), 8902-11

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

OS CJACS-IMAGE; CJACS

AB The authors are investigating an approach to protein recognition that is based on matching a pattern of metal ions in a synthetic receptor to a complementary pattern of metal-coordinating functional groups (histidine) on a protein's surface. In this model study, target "protein analogs" were constructed by linking two imidazoles via org. spacers of varying lengths. By computer modeling the individual targets and receptors, bis-Hg²⁺ receptors were designed to position two metal ions to match the available nitrogen ligands of their target bis-imidazoles. While ¹H NMR studies in DMSO-d₆ show that the receptors can bind 2 equiv of 1-benzylimidazole (K₁ .apprx. 10⁴ M⁻¹), a bis-imidazole is bound in a 1:1 complex with assocn. consts. as high as 3.times.10⁶ M⁻¹. Bis-metal ion receptors are indeed selective for their target bis-imidazoles in competitive binding expts., preferring the target over others that are both longer and shorter by .apprx.4 .ANG. (max. selectivity = 11.5). A max. selectivity of 140 was obsd. for the competition between a target bis-imidazole and 1-benzylimidazole. Increasing the available coordination sites on the metal ion significantly reduces selectivity, presumably by allowing the receptor to take on multiple bound conformations. Attempts to improve binding selectivity by restricting the receptors' conformational mobility reduced selectivity, primarily by introducing unanticipated unfavorable interactions with the target bis-imidazoles.

IT 147025-65-8P 147025-66-9P 158200-25-0P
158200-26-1P

(synthetic bis-metal ion receptors for bis-imidazole protein analogs)

L47 ANSWER 2 OF 10 CA COPYRIGHT 1995 ACS

AN 120:289504 CA

TI Highly potent and selective inhibition of human immunodeficiency virus by the bicyclam derivative JM3100

AU De Clercq, Erik; Yamamoto, Naohiko; Pauwels, Rudi; Balzarini, Jan; Witvrouw, Myriam; De Vreese, Karen; Debyser, Zeger; Rosenwirth, Brigitte; Peichl, Peter; et al.

CS Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain, B-3000, Belg.

SO Antimicrob. Agents Chemother. (1994), 38(4), 668-74

CODEN: AMACCQ; ISSN: 0066-4804

DT Journal

LA English

AB Bicyclams, in which the cyclam (1,4,8,11-tetraazacyclotetradecane) moieties are tethered via an aliph. bridge (i.e., propylene, as in JM2763) are potent and selective inhibitors of human immunodeficiency virus type 1 (HIV-1) and type-2 (HIV-2) (E. De Clercq, N. Yamamoto, R. Pauwels, M. Baba, D. Schols, H. Nakashima, J. Balzarini, Z. Debyser, B. A., Murrer, D. Schwartz, D. Thornton, G. Bridger, S. Fricker, G. Henson, M. Abrams, and D. Picker, Proc. Natl. Acad. Sci. USA 89:5286-5290, 1992). The authors have now found that the bicyclam JM3100, in which the cyclam moieties are tethered by an arom. bridge [i.e., phenylenebis(methylene)], inhibits the replication of various HIV-1 and HIV-2 strains in various cell lines at a 50% effective concn. (EC₅₀) of 1 to 10 ng/mL, which is about 100-fold lower than the concn. required for

JM2763 to inhibit HIV replication and at least 100,000-fold lower than the concn. required for JM2763 to inhibit HIV replication and at least 100,000-fold lower than the cytotoxic concn. (>500 $\mu\text{g/mL}$). In primary T4 lymphocytes or primary monocytes, JM3100 proved inhibitory to HIV-1 (IIIB) and several clin. HIV-1 isolated at an EC50 of less than 1 ng/mL. On the basis of time-of-addn. expts., JM3100 appeared to interact with a viral uncoating event, and this was further corroborated by an uncoating assay in which RNase sensitivity of [5-3H]uridine-labeled virions was monitored. In addn., but possibly mechanistically related, JM3100 blocks formation of infectious particles. JM3100 was also found to interfere directly with virus-induced syncytium formation, albeit at a higher concn. (1 to 2 $\mu\text{g/mL}$) than that required for inhibition of viral replication. Following s.c. injection of 10 mg of JM3100 per kg of body wt. to rabbits, anti-HIV activity was detected in serum corresponding to serum drug levels exceeding for at least 6 h by >100 -fold the EC50 required to inhibit HIV replication in vitro. When combined with either 3'-azido-2',3'-dideoxythymidine or 2',3'-dideoxyinosine, JM3100 achieved a additive inhibition of HIV replication, and when repeatedly subcultivated in the presence of JM3100, the virus remained insensitive to the compd. for at least 30 passages (120 days) in cell culture.

IT 155148-31-5

(HIV virus inhibition by, mechanism of, structure in relation to, in human cells)

IT 110078-44-9 151191-06-9 151191-09-2

155148-32-6

(HIV virus inhibition by, structure in relation to, in human cells)

L47 ANSWER 3 OF 10 CA COPYRIGHT 1995 ACS

AN 120:44414 CA

TI Functional group convergency in a binuclear dephosphorylation reagent

AU Vance, David H.; Czarnik, Anthony W.

CS Dep. Chem., Ohio State Univ., Columbus, OH, 43210, USA

SO J. Am. Chem. Soc. (1993), 115(25), 12165-6

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

OS CJACS-IMAGE; CJACS

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Phosphomonoesters experience rapid hydrolysis in the presence of 2 equiv of Co(III) complexes bearing substitutable cis-coordination sites. A binuclear Co(III) complex was synthesized possessing a phosphate-sized pocket, but rigidly so as to avoid μ -oxo dimer formation. X-ray anal. of the carbonato form I confirms the cofacial orientation of the metal centers, and ^{31}P NMR of the phosphate complex II suggests triscoordination of phosphate to Co(III). The binuclear complex at 1 mM affects the dephosphorylation of p-nitrophenyl phosphate 10-times faster than do

either the mononuclear Co(III)-cyclen or Co(III)-trpn complexes at 2 mM.

IT 151987-13-2P

(prepn. and crystal structure and aquation of)

IT 151697-44-8P

(prepn. and reaction of, with carbonatocobaltate)

IT 151956-64-8P

(prepn. and reaction with phosphate and catalysis by, of hydrolysis of phosphate esters)

L47 ANSWER 4 OF 10 CA COPYRIGHT 1995 ACS

AN 120:30786 CA

TI Linked heterocyclic polyamines with activity against HIV

IN Bridger, Gary James; Padmanabhan, Sreenivasan; Skerlj, Renato Tony; Thornton, David Michael

PA Johnson Matthey P.L.C., UK

SO PCT Int. Appl., 66 pp.

CODEN: PIXXD2

PI WO 9312096 A1 930624

DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AI WO 92-GB2334 921216

PRAI GB 91-26677 911216

DT Patent

LA English

OS MARPAT 120:30786

AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 = (un)substituted alk. chain or heteroatom-contg. chain; Y, Z = cyclic polyamine moieties having 9-32 ring members and 3-8 N atoms in the ring spaced by .gtoreq.2 C atoms from each other] or their acid addn. salts or metal complexes are prepd. and demonstrated viricidal activity against HIV-1 and HIV-2. Thus, 1,1'-[1,4-phenylenebis(methylene)]bis-1,4,8,11-tetraazacyclotetradecane was prepd. and demonstrated 50% inhibitory concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory concn. against HIV-2 of <0.01 .mu.g/mL in an assay employing infected MT-4 cells.

IT 151191-32-1 151191-33-2 151191-34-3

(HIV viricidal activity of)

IT 110078-44-9P 110078-46-1DP, copper and zinc complexes 151190-72-6P 151190-73-7P

151190-74-8P 151190-75-9P 151190-76-0P

151190-87-3P 151190-93-1P 151190-94-2P

151190-97-5P 151190-98-6P 151190-99-7P

151191-02-5P 151191-03-6P 151191-05-8P

151191-06-9P 151191-08-1P 151191-09-2P

151191-17-2P 151191-18-3P 151191-20-7P

151191-21-8P 151191-26-3P 151191-27-4P

151191-28-5P 151191-29-6P 151191-30-9P

151191-31-0P

(prepn. and HIV viricidal activity of)

IT 105355-16-6P 151190-70-4P 151190-71-5P

151190-86-2P 151190-92-0P 151191-01-4P

151191-04-7P 151191-07-0P 151191-16-1P

151191-19-4P

(prepn. and reaction of, in prepn. of heterocyclic HIV viricidal agents)

IT 110078-46-1

(reaction of, in prepn. of heterocyclic HIV viricidal agents)

L47 ANSWER 5 OF 10 CA COPYRIGHT 1995 ACS

AN 118:204007 CA

TI Selective recognition of bis-imidazoles by complementary bis-metal ion complexes

AU Mallik, Sanku; Johnson, Robert D.; Arnold, Frances H.

CS Div. Chem. Chem. Eng., California Inst. Technol., Pasadena, CA, 91125, USA

SO J. Am. Chem. Soc. (1993), 115(6), 2518-20
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

OS CJACS-IMAGE; CJACS

AB Metal ion complexes capable of selective recognition are made by matching the spatial distribution of metal ions in the complex to the spacing between coordinating ligands on the target mol. Two ligands (L), 1,4-di[(1',4',8',11'-tetraazacyclotetradecan-1'-yl)methylene]benzene (L1) and 2,6-di[(1',4',8',11'-tetraazacyclotetradecan-1'-yl)methylene]naphthalene (L2), were synthesized. The corresponding [Hg₂(H₂O)L](ClO₄) (3) were designed to bind a bis-imidazole target mol., 4,4'-di(imidazol-1-yl)methylenebiphenyl (2), preferentially over the closely related bis-imidazole, 1,4-di(imidazol-1-yl)xylene (1). From ¹H NMR chem. shifts in titrn. expts. 3 (L = L1) forms a cyclic complex with 2, but not with 1 in DMSO-d₆. Receptor 3 (L = L1) exhibits a selectivity of 10 in binding 2 over 1; the selectivity is increased to 14 with 3 (L = L2). This model system demonstrates that receptor complexes contg. properly-positioned metal ions can selectively bind target mols. with a complementary spatial distribution of metal-coordinating ligands. Metal ion complexes such as these may have applications as synthetic receptors for biol. mols. such as proteins that are characterized by unique pattern of surface coordinating ligands.

IT 110078-46-1DP, mercury dinuclear complexes with imidazole derivs. 147025-65-8DP, mercury dinuclear complexes with imidazole derivs.

(formation and binding selectivities of)

IT 147025-66-9P

(formation and deprotection of)

IT 147025-65-8P

(prepn. and reaction of, with mercury perchlorate)

L47 ANSWER 6 OF 10 CA COPYRIGHT 1995 ACS

AN 117:82274 CA

TI Synthesis and coordination chemistry of 1-(2',2''-bipyridyl-5'-yl-methyl)-1,4,8,11-tetraazacyclotetradecane L1. Quenching of fluorescence from [Ru(bipy)₂(L1)]²⁺ by coordination of Ni^{III} or Cu^{II} in the cyclam cavity (bipy = 2,2'-bipyridine; cyclam = 1,4,8,11-tetraazacyclotetradecane).

AU Rawle, Simon C.; Moore, Peter; Alcock, Nathaniel W.

CS Dep. Chem., Univ. Warwick, Coventry, CV4 7AL, UK

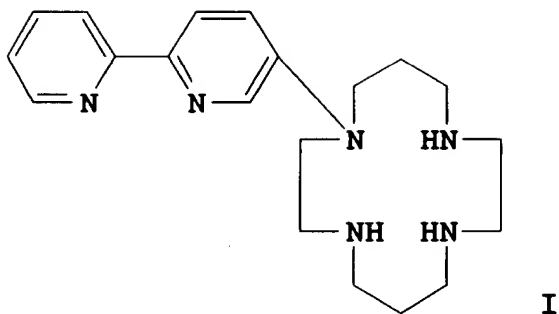
SO J. Chem. Soc., Chem. Commun. (1992), (9), 684-7
CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

LA English

OS CJRSC

GI

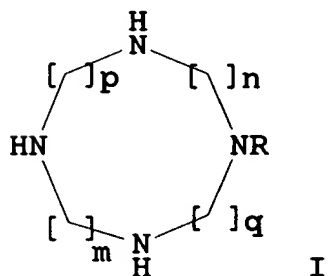


AB A novel bipy deriv. (I) of cyclam, designed for controlled and systematic polynuclear metal complex formation, is reported. Fluorescence quenching of the $[\text{Ru}(\text{bipy})_2]^{2+}$ core of $[(\text{bipy})_2\text{RuL}]^{2+}$ ($\text{L} = \text{I}$) upon coordination of CuII at the cyclam cavity is demonstrated. The crystal structure of $[\text{CuL}](\text{ClO}_4)_2 \cdot \text{MeNO}_2$ was detd.

IT 142079-95-6P
(prepn. of)

L47 ANSWER 7 OF 10 CA COPYRIGHT 1995 ACS
 AN 114:207294 CA
 TI Preparation of mono-N-substituted cyclic tetramines
 IN Handel, Henri; Yaouanc, Jean Jacques; Filali Zegzouti, Ayoub; Malouala, Denis; Des Abbayes, Herve; Clement, Jean Claude; Bernard, Helene; Le Gall, Guenaelle
 PA Centre National de la Recherche Scientifique, Fr.
 SO Eur. Pat. Appl., 20 pp.
 CODEN: EPXXDW
 PI EP 389359 A1 900926
 DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE
 AI EP 90-400762 900320
 PRAI FR 89-3600 890320
 DT Patent
 LA French
 OS MARPAT 114:207294
 GI

u, 5,047,527 x



AB The title compds. $[\text{I}; \text{R} = (\text{un})\text{satd. org. radical}; m-q = 2, 3; m = n = 2 \text{ and } p = 1 = 3; m = 2 \text{ and } n-q = 3; n = 2 \text{ and } m = p = q = 3; m = n$

= 3 and $p = q = 4$] were prepd. by substitution of I ($R = H$) in which 3 N-atoms are coordinated to a central group, e.g., $M(CO)_3$ ($M = Cr, Mo, W$). Thus, cyclam was refluxed 2-3 h with $Cr(CO)_6$ in deaerated Bu_2O and the product heated 2 h at 100.degree. with $PhCH_2Br$ in DMF contg. Na_2CO_3 to give I ($R = PhCH_2$; $m = n = 2, q = 3$).

IT 110078-44-9P 110078-46-1P 133563-60-7P
(prepn. of, method for)

L47 ANSWER 8 OF 10 CA COPYRIGHT 1995 ACS

AN 114:207229 CA

TI Mono N-functionalization of cyclic and linear tetraamines via their tridentate tricarbonylchromium complexes

AU Yaouanc, Jean Jacques; Le Bris, Nathalie; Le Gall, Guenaelle; Clement, Jean Claude; Handel, Henri; Des Abbayes, Herve

CS Fac. Sci. Tech., Brest, 29287, Fr.

SO J. Chem. Soc., Chem. Commun. (1991), (4), 206-7

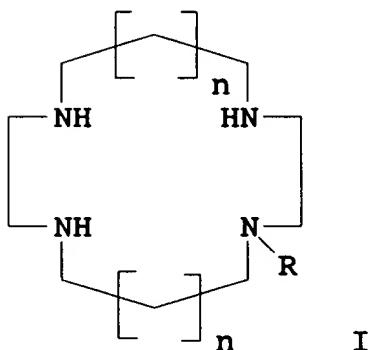
CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

LA English

OS CJRSC

GI



AB Cyclic tetraamines I ($R = H, n = 0, 1$) and $H_2N(CH_2)_nNHCH_2CH_2NH(CH_2)_nNH_2$ ($n = 2, 3$) were selectively monoalkylated in high yield at the uncomplexed N of a $Cr(CO)_3$ tridentate complex. Thus, I ($R = H$) upon treatment with $Cr(CO)_6$ in Bu_2O at 142.degree. gave 85-90% of a tridentate complex, which on treatment with $PhCH_2Br$ in DMF at 100.degree. followed by decomplexation afforded 85-95% ($R = CH_2Ph$).

IT 110078-44-9P 110078-46-1P

(prepn. of, by monoalkylation of tridentate chromium carbonyl complex)

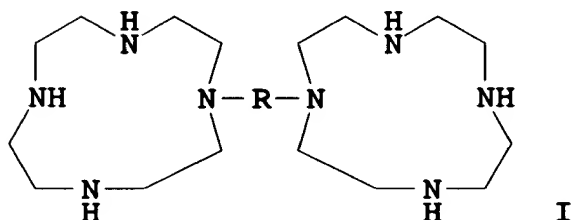
L47 ANSWER 9 OF 10 CA COPYRIGHT 1995 ACS

AN 107:167695 CA

TI Dinickel and dicopper complexes with N,N-linked bis(cyclam) ligands. An ideal system for the investigation of electrostatic effects on the redox behavior of pairs of metal ions

AU Ciampolini, Mario; Fabbrizzi, Luigi; Perotti, Angelo; Poggi, Antonio; Seghi, Barbara; Zanolini, Fabrizio

CS Dip. Chim. Gen., Univ. Pavia, Pavia, 27100, Italy
SO Inorg. Chem. (1987), 26(21), 3527-33
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
OS CJACS
GI



AB I (R = (CH₂)₂, (CH₂)₃, (CH₂)₄, m-xyllyl, p-xyllyl) were prepd. by condensation of N,N',N''-tritosylcyclam (2 equiv) with an XRX fragment (X = Br or OTs). M₂L₄⁺ (M = Ni, Cu; H₄L = I) undergo a 2-electron-oxidn. process, according to 2 reversible 1-electron steps, whose redox potentials are sepd. by the quantity .DELTA.E.degree.. The value of .DELTA.E is related to the comproportionation (or valence scrambling) equil. [MIIIMIIL]₆⁺ + [MIIMIIL]₄⁺ .dblharw. 2[MIIIMIIL]₅⁺ and results from the combination of a statistical fixed contribution and a term that reflects the electrostatic repulsion between the metal centers of the dinuclear complex. The electrostatic repulsion term decreases when the distance between the metal centers is increased, according to a hyperbolic mode, but does not show any definite dependence upon the macroscopic values of the dielec. const. of the explored media. Moreover, the electrostatic term significantly varies with the stereochem. features of each metal center in its oxidn. state (II or III), which cannot be any longer considered as simple point charges.

IT 110078-45-0P 110078-47-2P
(prepn. and detosylation of)

IT 110078-44-9P 110078-46-1P
(prepn. of)

L47 ANSWER 10 OF 10 CA COPYRIGHT 1995 ACS

AN 106:26833 CA

TI Metal complexes with macrocyclic ligands. Part XXII. Synthesis of two bis(tetraaza)macrocycles and study of the structures, electrochemistry, visible and ESR spectra of their binuclear copper(2+) and nickel(2+) complexes

AU Schneider, Rene; Riesen, Andreas; Kaden, Thomas A.

CS Inst. Anorg. Chem., Univ. Basel, Basel, CH-4056, Switz.

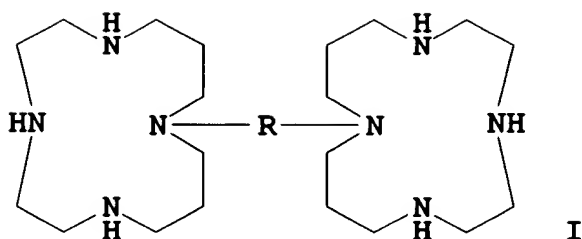
SO Helv. Chim. Acta (1986), 69(1), 53-61

CODEN: HCACAV; ISSN: 0018-019X

DT Journal

LA English

GI



AB I (R = p-CH₂C₆H₄CH₂, CH₂CH₂) were prep'd. by 1,4,7-tritosyl-1,4,7,11-tetraazacyclotetradecane as starting comp'd. and bifunctional alkylating agents. The bis-macrocycles give binuclear complexes with Ni²⁺ and Cu²⁺, the properties of which were studied to obtain information about the interaction of the 2 subunits as a function of the distance. The visible spectra of the Ni²⁺ and Cu²⁺ complexes indicate that both metal ions are in a square-planar geometry as expected from the result of the analogous complexes with 1,4,7,11-tetraazacyclotetradecane. Cyclic voltammetry and differential pulse polarog. of the binuclear Ni²⁺ complexes in CH₃CN show a single 2-electron step for I (R = CH₂CH₂), whereas 2 distinct 1-electron redox processes can be obsd. for I (R = p-CH₂C₆H₄CH₂), indicating that the 2 metal ions interact with each other when the chain length is shorter. Similarly, the EPE studies of frozen solns. of the binuclear Cu²⁺ complexes clearly show that a magnetic dipolar interaction between the 2 paramagnetic centers exists, and that the strength of it depends upon the length of the bridge. Finally, from the x-ray structures of the binuclear Ni²⁺ complexes with I, 2 rings are kept apart as far as possible; the distances between the two metal ions detd. in the solid correlate well with the observation in soln.

IT 105355-16-6P

(prepn. and deblocking of)

IT 105390-46-3P

(prepn. of)